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Surface chemical analysis — Vocabulary —

Part 1:
General terms and terms used in spectroscopy

Analyse chimique des surfaces — Vocabulaire —

Partie 1: Termes généraux et termes utilisés en spectroscopie

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ISO copyright office
CP 401 • Ch. de Blandonnet 8
CH-1214 Vernier, Geneva
Phone: +41 22 749 01 11
Email: copyright@iso.org
Website: www.iso.org

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Foreword

ISO (the International Organization for Standardization) is a worldwide federation of national standards bodies (ISO member bodies). The work of preparing International Standards is normally carried out through ISO technical committees. Each member body interested in a subject for which a technical committee has been established has the right to be represented on that committee. International organizations, governmental and non-governmental, in liaison with ISO, also take part in the work. ISO collaborates closely with the International Electrotechnical Commission (IEC) on all matters of electrotechnical standardization.

The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO documents should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 201, *Surface chemical analysis*, Subcommittee SC 1, *Terminology*.

This third edition cancels and replaces the second edition (ISO 18115-1:2013), which has been technically revised.

The main changes are as follows:

- revision of definitions related to resolution;
- introduction of definitions related to atom probe tomography;
- introduction of emerging methods such as HAXPES, NAPXPS, GEXRF;
- removal of repeated or redundant definitions and references;
- reorganisation of the terminology into subject-specific sections;
- removal of Annexes according to ISO requirements.

A list of all parts in the ISO 18115 series can be found on the ISO website.

Any feedback or questions on this document should be directed to the user's national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

Surface chemical analysis is an important area which involves interactions between people with different backgrounds and from different fields. Those conducting surface chemical analysis can be materials scientists, chemists, or physicists and can have a background that is primarily experimental or primarily theoretical. Those making use of the surface chemical data extend beyond this group into other disciplines.

With the present techniques of surface chemical analysis, compositional information is obtained for regions close to a surface (generally within 20 nm) and composition-versus-depth information is obtained with surface analytical techniques as surface layers are removed. The surface analytical terms covered in this document extend from the techniques of electron spectroscopy and mass spectrometry to optical spectrometry and X-ray analysis. The terms covered in ISO 18115-2 relate to scanning-probe microscopy. The terms covered in ISO 18115-3 relate to optical interface analysis. Concepts for these techniques derive from disciplines as widely ranging as nuclear physics and radiation science to physical chemistry and optics.

The wide range of disciplines and the individualities of national usages have led to different meanings being attributed to particular terms and, again, different terms being used to describe the same concept. To avoid the consequent misunderstandings and to facilitate the exchange of information, it is essential to clarify the concepts, to establish the correct terms for use, and to establish their definitions.

The terms are classified under Clauses 3 to 22:

- Clause 3: Terms related to general concepts in surface chemical analysis;
- Clause 4: Terms related to particle transport in materials;
- Clause 5: Terms related to the description of samples;
- Clause 6: Terms related to sample preparation;
- Clause 7: Terms related to instrumentation;
- Clause 8: Terms related to experimental conditions;
- Clause 9: Terms related to sputter depth profiling;
- Clause 10: Terms related to resolution;
- Clause 11: Terms related to electron spectroscopy methods;
- Clause 12: Terms related to electron spectroscopy analysis;
- Clause 13: Terms related to X-ray fluorescence, reflection and scattering methods;
- Clause 14: Terms related to X-ray fluorescence, reflection and scattering analysis;
- Clause 15: Terms related to glow discharge methods;
- Clause 16: Terms related to glow discharge analysis;
- Clause 17: Terms related to ion scattering methods;
- Clause 18: Terms related to ion scattering analysis;
- Clause 19: Terms related to surface mass spectrometry methods;
- Clause 20: Terms related to surface mass spectrometry analysis;
- Clause 21: Terms related to atom probe tomography;
- Clause 22: Terms related to multivariate analysis.

Surface chemical analysis — Vocabulary —

Part 1:
General terms and terms used in spectroscopy

1 Scope

This part of the ISO 18115 series defines terms for surface chemical analysis. It covers general terms and those used in spectroscopy, while ISO 18115-2 covers terms used in scanning-probe microscopy and ISO 18115-3 covers terms used in optical interface analysis.

2 Normative references

There are no normative references in this document.

3 Terms related to general concepts in surface chemical analysis

ISO and IEC maintain terminology databases for use in standardization at the following addresses:

- ISO Online browsing platform: available at https://www.iso.org/obp
- IEC Electropedia: available at https://www.electropedia.org/

3.1
interface
boundary between two phases having different chemical, elemental, or physical properties

3.2
surface
interface (3.1) between a condensed phase and a gas, vapour, or free space

3.3
measurand
quantity intended to be measured

[SOURCE: ISO/IEC Guide 99:2007,[1] 2.3, modified — The notes to entry have been deleted.]

3.4
analyte
substance or chemical constituent that is subjected to measurement

3.5
chemical species
atom, molecule, ion, or functional group

3.6

unified atomic mass unit

u

dalton

Da

unit equal to 1/12 of the mass of the nuclide ^{12}C at rest and in its ground state

Note 1 to entry: 1 u ≈ 1,660 538 86 × 10^{-27} kg with a one-standard-deviation uncertainty of ±0,000 000 28 × 10^{-27} kg.[2] This is a non-SI unit, accepted for use with the International System, whose value in SI units is obtained experimentally.

Note 2 to entry: The term dalton, symbol Da, is preferred over unified atomic mass unit as it is both shorter and works better with prefixes.

Note 3 to entry: The above definition was agreed upon by the International Union of Pure and Applied Physics in 1960 and the International Union of Pure and Applied Chemistry in 1961, resolving a longstanding difference between chemists and physicists. The unified atomic mass unit replaced the atomic mass unit (chemical scale) and the atomic mass unit (physical scale), both having the symbol amu. The amu (physical scale) was one-sixteenth of the mass of an atom of oxygen-16. The amu (chemical scale) was one-sixteenth of the average mass of oxygen atoms as found in nature. In the 1998 CODATA, 1 u = 1,000 317 9 amu (physical scale) = 1,000 043 amu (chemical scale).

3.7

reference method

thoroughly investigated method, clearly and exactly describing the necessary conditions and procedures for the measurement of one or more property values, that has been shown to have accuracy and precision commensurate with its intended use and that can therefore be used to assess the accuracy of other methods for the same measurement, particularly in permitting the characterization of a *reference material* (5.1)

[SOURCE: ISO Guide 30:1992+A1:2008[3]]

3.8

quantitative analysis

determination of the amount of *analyte* (3.4) detected in, or on, a sample

Note 1 to entry: The analytes can be elemental or compound in nature.

Note 2 to entry: The amounts can be expressed, for example, as atomic or mass percent, atomic or mass fraction, mole or mass per unit volume, as appropriate or as desired.

Note 3 to entry: The sample material can be inhomogeneous so that a particular model structure may be assumed in the interpretation. Details of that model should be stated.

3.9

detection limit

smallest amount of an element or compound that can be measured under specified analysis conditions

Note 1 to entry: The detection limit is often taken to correspond to the amount of material for which the total signal for that material minus the *background signal* (3.21) is three times the standard deviation of the signal above the background signal. This approach is simplistic and, for more accurate and rigorous definitions of detection limits, the References [4] and [5] should be consulted.

Note 2 to entry: The detection limit can be expressed in many ways, depending on the purpose. Examples of ways of expressing it are mass or weight fraction, atomic fraction, concentration, number of atoms, and mass or weight.

Note 3 to entry: The detection limit is generally different for different materials.

3.10

matrix effects

change in the intensities or spectral information per atom of the *analyte* (3.4) arising from change in the chemical or physical environment

Note 1 to entry: Examples of these environments are varying sample morphologies [e.g. *thin films* (5.13), clusters, fibres, nanostructures] of different dimensions, the amorphous or crystalline state, changes of matrix species, and the proximity of other physical phases or *chemical species* (3.5).

3.11

matrix factor

factors, arising from the composition of the matrix, for multiplying the quotient of the measured intensity and the appropriate sensitivity factor in formulae to determine the composition using surface analytical techniques

Note 1 to entry: See average matrix sensitivity factor and pure-element sensitivity factor.

Note 2 to entry: In methods such as *AES* (11.1), the matrix factor is determined in part by the composition of the sub-surface material and in part by the composition of the *analysis volume* (8.48) in the sample.

3.12

absolute elemental sensitivity factor

coefficient for an element by which the measured intensity for that element is divided to yield the atomic concentration or atomic fraction of the element present in the sample

Note 1 to entry: See *elemental relative sensitivity factor* (12.92) (20.61).

Note 2 to entry: The choice of atomic concentration or atomic fraction should be made clear.

Note 3 to entry: The type of sensitivity factor utilized should be appropriate for the formulae used in the quantification process and for the type of sample analysed, for example homogeneous samples or segregated layers.

Note 4 to entry: The source of sensitivity factors should be given to ensure that the correct *matrix factors* (3.11) or other parameters are used.

Note 5 to entry: Sensitivity factors depend on parameters of the excitation source, the spectrometer, and the orientation of the sample to these parts of the instrument. Sensitivity factors also depend on the matrix being analysed, and in *SIMS* (19.1) this has a dominating influence.

3.13

step size

distance between values in *measurand* (3.3) space from which individual data points are acquired

3.14

sweep

single, complete acquisition of one set of data

3.15

peak intensity

measure of *signal intensity* (3.17) for a constituent spectral peak

Note 1 to entry: Intensity is usually measured for quantitative purposes which can be the height of the peak above a defined background or the *peak area* (3.16). The units can be *counts* (3.18), counts·electron volts, counts per second, counts·electron volts per second, counts per amu, counts per second per amu, etc. For differential spectra, the intensity can be the peak-to-peak height or the peak-to-background height. The measure of intensity should be defined and the units stated in each case.

Note 2 to entry: The meaning is very rarely the literal meaning of the intensity value at the top of the measured peak either before or after removal of any background.

3.16
peak area
area under a peak in a spectrum after background removal

Note 1 to entry: See *inelastic electron scattering background subtraction* (12.85) and *signal intensity* (3.17).

Note 2 to entry: The peak area can be expressed in *counts* (3.18), counts·electron volts, counts·electron volts per second, counts per amu, or other units.

3.17
signal intensity
strength of a measured signal at a spectrometer detector or after some defined processing

Note 1 to entry: The signal intensity is subject to significant change between the points of generation and detection of the signal and, further, between the points of detection and display on the measuring instrument.

Note 2 to entry: The signal intensity can be expressed in *counts* (3.18) (per channel) or counts per second (per channel) or counts·electron volts per second or other units. In *AES* (11.1), the differential of the signal intensity may be obtained by analogue *modulation* (12.61) of an electrode in the spectrometer or by numerical differentiation of the spectrum. The type of signal shall be defined.

Note 3 to entry: In an electron or *mass spectrum* (20.58), the measured spectrum integrated over energy or mass and solid angle is equal to a current. If the spectrometer has been calibrated, the units of intensity can be current·eV^{-1}·sr^{-1} or current·amu^{-1}·sr^{-1}. If the spectrum has been normalized to unit *primary-beam* (8.10) current, the appropriate units would be eV^{-1}·sr^{-1} or amu^{-1}·sr^{-1}. If the spectrum has also been integrated over the emission solid angle, the appropriate units would be eV^{-1} or amu^{-1}.

3.18
counts
total number of pulses recorded by a detector system in a defined time interval

Note 1 to entry: The counts can be representative, one-for-one with the particles being detected [in the absence of *dead time* (7.17) losses in the counting measurement] in which case they follow Poissonian statistics [unless other *noise* (3.19) sources are present] or they can simply be proportional to the number of particles being detected. The type of measure shall be clearly stated.

Note 2 to entry: In multidetector systems, the apportion of counts into relevant channels of the spectrum can lead to changes from the expected Poissonian statistics in each channel since the counts in neighbouring channels can be partly correlated.

3.19
noise
time-varying disturbances superimposed on the analytical signal with fluctuations, leading to uncertainty in the *signal intensity* (3.17)

Note 1 to entry: An accurate measure of noise can be determined from the standard deviation of the fluctuations. Visual or other estimates, such as peak-to-peak noise in a spectrum, can be useful as semiquantitative measures of noise.

Note 2 to entry: The fluctuations in the measured intensity can arise from a number of causes, such as *statistical noise* (3.20) and electrical interference.

3.20
statistical noise
noise (3.19) in the spectrum due solely to the statistics of randomly detected single events

Note 1 to entry: For single-particle counting systems exhibiting Poisson statistics, the standard deviation of a large number of measures of an otherwise steady count rate, *N*, each in the same time interval, is equal to the square root of *N*.

Note 2 to entry: In multidetector systems, the data processing required to generate the output spectrum can lead to statistical correlation between adjacent channels and also an apparent noise in each channel that is less than Poissonian.

3.21
background signal

signal present at a particular position, energy, mass or wavelength due to processes or sources other than those of primary interest

Note 1 to entry: See *metastable background* (20.36), *Shirley background* (12.86), *Sickafus background* (12.87), and *Tougaard background* (12.88).

3.22
peak-to-background ratio

signal-to-background ratio

ratio of the maximum height of the peak above the background intensity to the magnitude of that background intensity

Note 1 to entry: Signal-to-background ratio is the more commonly used term in *GDS* (15.1), where it is abbreviated to SBR. Peak-to-background ratio is the more commonly used term for types of electron spectroscopies such as *AES* (11.1) and *XPS* (11.6).

Note 2 to entry: The method of estimating the background intensity shall be given. For AES, the background intensity is often determined at a *kinetic energy* (3.35) just above the peak of interest.

3.23
signal-to-noise ratio

ratio of the *signal intensity* (3.17) to a measure of the total *noise* (3.19) in determining that signal

Note 1 to entry: See *statistical noise* (3.20).

Note 2 to entry: The noise in *AES* (11.1) is often measured at a convenient region of the spectral background close to the peak.

3.24
smoothing

mathematical treatment of data to reduce the apparent *noise* (3.19)

3.25
interference signal

<mass spectrometry, spectroscopy> signal, measured at the mass, energy, or wavelength position of interest, due to another, undesired, species

Note 1 to entry: In general laboratory use, interference can be used more broadly to indicate electrical *noise* (3.19), line pick-up, or other unwanted contributions to the detected signal.

3.26
relative standard deviation of the background

quotient of the standard deviation characterizing the *noise* (3.19) in the *background signal* (3.21) by the intensity of the background signal

3.27
lineshape

measured shape of a particular spectral feature

3.28
peak width

width of a peak at a defined fraction of the peak height

Note 1 to entry: See *intrinsic linewidth* (12.22).

Note 2 to entry: Any background subtraction method used should be specified.

Note 3 to entry: The most common measure of peak width is the full width of the peak at half maximum (FWHM) intensity.

Note 4 to entry: For asymmetrical peaks, convenient measures of peak width are the half-widths of each side of the peak at half maximum intensity.

3.29
peak fitting
procedure whereby a spectrum, generated by *peak synthesis* (3.30), is adjusted to match a measured spectrum

Note 1 to entry: A least-squares optimization procedure is generally used in a computer programme for this purpose.

Note 2 to entry: The selected peak shape and the background shape should be defined. Any constraints imposed on the adjustment process should also be defined.

3.30
peak synthesis
procedure whereby a synthetic spectrum is generated, using either model or experimental peak shapes, in which the number of peaks, the peak shapes, the *peak widths* (3.28), the peak positions, the peak intensities, and the background shape and intensity are adjusted for *peak fitting* (3.29)

Note 1 to entry: The selected peak shape and the background shape should be defined.

3.31
lateral profile
chemical or elemental composition, *signal intensity* (3.17) or processed intensity information from the available software measured in a specified direction parallel to the *surface* (3.2)

Note 1 to entry: See *line scan* (8.56).

3.32
depth profile
vertical profile
chemical or elemental composition, *signal intensity* (3.17) or processed intensity information from the available software measured in a direction normal to the *surface* (3.2)

Note 1 to entry: See *compositional depth profile* (3.33).

3.33
compositional depth profile
CDP
atomic or molecular composition measured as a function of distance normal to the *surface* (3.2)

3.34
depth profiling
monitoring of *signal intensity* (3.17) as a function of a variable that can be related to distance normal to the *surface* (3.2)

Note 1 to entry: See *compositional depth profile* (3.33).

Note 2 to entry: In a *sputter depth profile* (9.1) the signal intensity is usually measured as a function of the *sputtering* (9.3) time.

3.35
kinetic energy
energy of motion

Note 1 to entry: The energy of a charged particle due to motion is not necessarily constant and varies with the local electric potential. If all local electrodes are at ground potential, the kinetic energy of the particle varies with the local *vacuum level* (12.10). This vacuum level can vary over a range of 1 eV in different regions of *AES* (11.1) and *XPS* (11.6) instruments and measured electron energies can similarly vary. This variation is removed if the kinetic energies are referred to the *Fermi level* (12.9). In XPS, by convention, the Fermi level is always used but in AES both *vacuum* (12.76) and *Fermi level referencing* (12.75) are practised. Instruments capable of both AES and XPS are Fermi level referenced. Fermi level referencing is recommended for accurate measurements of energies in AES. In *electron spectrometers* (12.58), Fermi level referenced energies are typically 4,5 eV greater than those referenced to the vacuum level. It is convenient in AES to assume a *standard vacuum level* (12.11) of 4,500 eV above the Fermi level so that the energies of *Auger electron* (12.32) peaks, referenced to the Fermi level, can be converted in a consistent way to energies referenced to the vacuum level and vice versa.

3.36
ion species
type and charge of an ion

EXAMPLE Ar$^+$, O$^-$, and H_2^+.

Note 1 to entry: If an isotope is used, it should be specified.

3.37
radical
atoms or molecular entity possessing an unpaired electron

Note 1 to entry: Entities such as $^{\bullet}CH_3$, $^{\bullet}SnH_3$, and $Cl^{\bullet}$ have formulae in which the dot symbolizing the unpaired electron is placed so as to indicate the atom of highest spin density, if this is possible. Paramagnetic metal ions are not normally regarded as radicals.

Note 2 to entry: Depending upon the core atom that possesses the unpaired electron, the radicals can be described as carbon-, oxygen-, nitrogen-, or metal-centred radicals. If the unpaired electron occupies an orbital having considerable “s” or more or less pure “p” character, the respective radicals are termed σ- or π-radicals.

Note 3 to entry: The adjective “free” is no longer used.

3.38
radical ion
radical (3.37) carrying an electric charge

Note 1 to entry: A positively charged radical is called a “radical cation” (e.g. the benzene radical cation $C_6H_6^{\bullet +}$); a negatively charged radical is called a “radical anion” (e.g. the benzene radical anion $C_6H_6^{\bullet -}$ or the benzophenone radical anion $Ph_2C{-}O^{\bullet -}$). Commonly, but not necessarily, the odd electron and the charge are associated with the same atom. Unless the positions of unpaired spin and charge can be associated with specific atoms, superscript dot and charge designations should be placed in the order •+ or •− as suggested by the name “radical ion” (e.g. $C_3H_6^{\bullet +}$).

3.39
light ion
ion lighter than lithium

Note 1 to entry: See *intermediate-mass ion* (3.40) and *heavy ion* (3.41).

3.40
intermediate-mass ion
ion with mass between, and including, lithium and argon

Note 1 to entry: See *heavy ion* (3.41) and *light ion* (3.39).

3.41

heavy ion

ion heavier than argon

Note 1 to entry: See *intermediate-mass ion* (3.40) and *light ion* (3.39).

3.42

anion

negatively charged ion

Note 1 to entry: See *cation* (3.43).

3.43

cation

positively charged ion

Note 1 to entry: See *anion* (3.42) and *cationized molecule* (20.22).

3.44

cluster ion

ion composed of many atoms or *chemical species* (3.5)

Note 1 to entry: The cluster can have a positive or negative charge.

Note 2 to entry: Cluster ions are used to desorb molecular species from surfaces with enhanced efficiencies. Examples include ions produced in liquid metal sources (Au_n^+, Bi_n^+) as well as ions produced by electron impact [C_{60}^+, $Ar_n^+ (H_2O)_n^+$].

3.45

ionization efficiency

ratio of the number of ions formed to the number of electrons, ions, or photons used in an ionization process

[SOURCE: IUPAC]

3.46

ion neutralization

<ISS, SIMS> *charge exchange* (16.35) process in which an ion loses its charge through interactions with a material *surface* (3.2) or with gas-phase atoms or molecules

3.47

de Broglie wavelength

wavelength of a particle deduced from de Broglie's concept of wave-particle duality

Note 1 to entry: The wavelength is calculated as the quotient of Planck's constant and the particle momentum.

3.48

energy eigenvalue

energy value of a single bound electron level in an atom, molecule, ion, or solid obtained by solving the single-electron Schrödinger or Dirac formula in the Dirac-Fock representation of the electronic structure of an atom in its ground state

Note 1 to entry: Eigenvalues are the solutions to certain integral formulae, a special case of which is the Schrödinger formula for electrons in atoms, molecules, ions, or solids.

Note 2 to entry: In the *frozen-orbital approximation* (3.49), the *binding energy* (12.16) of a *hole state* (3.62) is given by the negative of the corresponding single-electron energy eigenvalue.

3.49
frozen-orbital approximation
assumption that the one-electron wavefunctions of the electrons remaining in an atom or molecule are unchanged after ionization

Note 1 to entry: In the frozen-orbital approximation, the *binding energy* (12.16) of an electron is given by the negative of the *energy eigenvalue* (3.48).

3.50
Koopmans energy
calculated energy of an electron in an orbital, on the assumption that its removal to infinity is unaccompanied by *electronic relaxation* (3.58)

3.51
orbital energy
<XPS> *Koopmans energy* (3.50) corrected for intra-atomic *relaxation* (3.57)

3.52
spin orbit splitting
splitting of p, d, or f levels in an atom arising from coupling of the spin and orbital angular momentum

3.53
excited state
state of a system with energy higher than that of the ground state

Note 1 to entry: This term is generally used to characterize a molecule in one of its electronically excited states, but can also refer to vibrational and/or rotational excitation in the electronic ground state.

3.54
initial state
<AES> core-hole *excited state* (3.53) of an atom prior to an *Auger transition* (12.33) or to X-ray emission

3.55
initial state
<XPS> ground state of an atom prior to photoelectron emission

3.56
final state
<AES, XPS> state of an atom resulting after a particular Auger, X-ray, or *photoemission* (12.8) process

3.57
relaxation
process by which an atom, molecule, or ion is transformed from a higher potential-energy state to a lower potential-energy state

Note 1 to entry: See *electronic relaxation* (3.58).

3.58
electronic relaxation
relaxation (3.57) resulting from the transition of an electron between energy levels, resulting in the release of energy

Note 1 to entry: The energy release can result in the ejection of a photon or other particle.

3.59
relaxation energy
<XPS> energy associated with intra-atomic or extra-atomic electronic readjustment to the removal of an atomic electron, so as to minimize the energy of the final state (3.56) of the system

3.60

extra-atomic relaxation energy

screening energy

diminished energy of an ionized atom in a solid due to coulombic attraction of electrons in the immediate environment

3.61

hole

electronic vacancy in an atom, molecule, or solid

3.62

hole state

electronic configuration of an atom, molecule, or solid containing a *hole* (3.61)

3.63

spectator hole

hole state (3.62) in the electronic structure of an atom that can be present during processes such as *Auger electron* (12.32) and X-ray photoelectron emission but is not created or destroyed in the process

3.64

X-ray fluorescence

<AES, TXRF, XPS> X-rays generated by a transition of an electron from a filled shell to a core *hole* (3.61), created by incident radiation, at a higher *binding energy* (12.16)

3.65

fluorescence yield

<AES, TXRF, XPS> probability that an atom with a vacancy in a particular inner shell relaxes by X-ray *fluorescence* (3.64)

3.66

characteristic X-rays

photons emitted by ionized atoms and having a particular distribution in energy and intensity which is characteristic of the atomic number and chemical environment of the atom

Note 1 to entry: In *XPS* (11.6), the term is applied to the X-ray source used to excite photoelectrons in the sample.

Note 2 to entry: In electron probe microanalysis, characteristic X-rays emitted from the sample are detected and analysed to give information on the composition of the sample.

3.67

X-ray linewidth

energy width of the principal *characteristic X-ray* (3.66) line

Note 1 to entry: In *XPS* (11.6) the X-ray linewidth usually refers to that of the X-ray source.

Note 2 to entry: The X-ray linewidth contributes to the photoelectron *peak widths* (3.28).

3.68

X-ray monochromator

device used to eliminate photons of energies other than those in a narrow energy or wavelength band

3.69

ion lifetime

average time that an ion exists in a particular electronic configuration, for example as a vacancy in a particular shell of an atom

3.70

Auger de-excitation

process in which the excess energy of an excited atom or ion is given up by the *Auger process* (12.30)

Note 1 to entry: See *Auger neutralization* (3.71).

Note 2 to entry: The Auger process can involve energy levels in neighbouring atoms and lead to ejection of an electron into the vacuum. This electron's energy can then usefully be characteristic of a surface atom with which a metastable probe atom (e.g. He) is in close proximity.

3.71

Auger neutralization

<ion at a surface> process in which an electron, tunnelling from the conduction band of a solid, neutralizes an incoming ion and an electron is ejected from a surface atom

Note 1 to entry: The ejected electron can be emitted into the vacuum.

3.72

time constant

<analogue electronic circuits> time required for a signal to change by [1 − (1/e)], or 63,2 %, of its final value in response to a step function input

3.73

sum rule

<dielectric function> formula that gives the value of an integral of a specified dielectric function

Note 1 to entry: Formulae have been derived that give expected values of integrals of the imaginary part of the complex dielectric constant and of the imaginary part of the reciprocal of the complex dielectric constant for any material. The integrals involve the product of the specified dielectric function and either frequency or inverse frequency from zero frequency to an infinite frequency. The values of each integral can be used to assess the internal consistency of a set of dielectric data for a material by comparing values of the specified integrals to expected values. In practice, the integrations are made from low frequencies (corresponding to infrared or visible photon energies) to frequencies much higher than those corresponding to the largest K-shell *binding energy* (12.16) of atoms in the material.

Note 2 to entry: The integral of the product of the specified dielectric function and frequency is proportional to the total number of electrons per atom or molecule in the material. This sum rule is often referred to as the f-sum rule, the oscillator-strength sum rule, or the Thomas-Reiche-Kuhn sum rule.

4 Terms related to particle transport in materials

4.1

binary elastic scattering

elastic scattering

collision between a moving particle and a second particle in which the total *kinetic energy* (3.35) and the total momentum are conserved

Note 1 to entry: See *inelastic scattering* (4.2).

Note 2 to entry: In elastic scattering interactions, the moving particle can be deflected through angles of up to 180°.

4.2

inelastic scattering

interaction between a moving energetic particle and a second particle or assembly of particles in which the total *kinetic energy* (3.35) is not conserved

Note 1 to entry: Kinetic energy is absorbed in solids by various mechanisms, for example inner-shell ionization, *plasmon* (12.47) and phonon excitation, and *bremsstrahlung* (12.57) generation. These excitations usually lead to a small change in direction of the moving particle.

Note 2 to entry: In particle collisions, the collision can be elastic in that the kinetic energy of the particles is conserved, but energy can still be lost by the incident particle. In the scattering of electrons by atoms, the energy lost is usually very small and is often ignored. Where it is not ignored, the scattering is often termed quasi-elastic [see *elastic peak* (12.42)].

4.3
energy loss
energy dissipated by particles as they interact with the sample

Note 1 to entry: See *characteristic electron energy losses* (12.40) and *plasmon* (12.47).

4.4
backscattering energy
energy of a particle from the *primary beam* (8.10) after it has undergone a backscattering collision and escaped from the sample

4.5
Bohr's critical angle
angle of ion scattering from a nucleus given by the ratio of the *de Broglie wavelength* (3.47) and the distance of closest approach of the ion with the nucleus

Note 1 to entry: Quantum effects are usually ignored for *scattering angles* (8.4) larger than Bohr's critical angle. For surface analysis conditions, this angle is very small.

4.6
Compton scattering
scattering of X-rays and other photons by electrons

Note 1 to entry: The photon loses energy by recoil of the electron to an extent governed by the *scattering angle* (8.4).

4.7
cross section
<for a specified target entity and for a specified reaction or process produced by incident charged or uncharged particles of specified type and energy> quotient of the probability of reaction or process for the target entity by the incident-particle *fluence* (8.16)

Note 1 to entry: Cross sections are often expressed as an area per target entity (atom, molecule, etc.) for the relevant process.

Note 2 to entry: A cross section of σ per atom for the removal of particles from a given state in a beam leads to a reduction dN in the number N of particles in that state in a distance dx, given by the relationship:

$$\mathrm{d}N = N\sigma n\,\mathrm{d}x$$

where n is the density of atoms traversed by the beam.

Integration leads to the relationship

$$N = N_\mathrm{o}\exp\left(-n\sigma x\right)$$

where N_o is the value of N at the origin of x.

4.8
elastic scattering cross section
cross section (4.7) for *binary elastic scattering* (4.1)

4.9
differential elastic scattering cross section
quotient of the *elastic scattering cross section* (4.8) for scattering into a particular infinitesimal solid angle far from the *target* (18.2) by that infinitesimal solid angle

Note 1 to entry: The differential elastic scattering cross section is related to the elastic scattering cross section, σ_e, by

$$\sigma_\mathrm{e} = \int_{4\pi} \frac{\mathrm{d}\sigma_\mathrm{e}(\Omega)}{\mathrm{d}\Omega}\mathrm{d}\Omega$$

where $\mathrm{d}\sigma_\mathrm{e}(\Omega)/\mathrm{d}\Omega$ is the differential elastic scattering cross section for scattering into solid angle Ω.

4.10
transport cross section

σ_tr

quotient of the fractional momentum loss of a particle incident on the sample arising from *elastic scattering* (4.1) by the areic density of the sample atoms, for an infinitesimally thin sample

Note 1 to entry: This *cross section* (4.7) is expressed as an area per atom.

Note 2 to entry: The cross section for the loss of any momentum, however small, is simply the *elastic scattering cross section* (4.8). By contrast, the transport cross section is a measure of the probability of the loss of a substantial fraction of the initial momentum, analogous to *stopping cross section* (4.11) which is a measure of the probability of the loss of a substantial amount of energy.

Note 3 to entry: The transport cross section is related to the *differential elastic scattering cross section* (4.9), $\mathrm{d}\sigma_\mathrm{e}(\Omega)/\mathrm{d}\Omega$, by

$$\sigma_\mathrm{tr} = 2\pi \int_0^\pi \frac{\mathrm{d}\sigma_\mathrm{e}(\Omega)}{\mathrm{d}\Omega}(1-\cos\theta)\sin\theta\,\mathrm{d}\theta$$

where θ is the *angle of scattering* (8.4).

4.11
stopping cross section

<ISS, RBS, sputtering> quotient of the rate of *energy loss* (4.3) of a particle with distance along its trajectory in a sample by the atomic density of sample atoms for an infinitesimal sample thickness

Note 1 to entry: See *stopping power* (4.17).

Note 2 to entry: The stopping cross section is usually expressed in units of eV·m^2 per atom and not as an area per atom as is customary for *cross sections* (4.7).

Note 3 to entry: The atomic density is usually taken as the number density, N, but sometimes as the mass density, ρ, so that the units are eV·m^2/atom or eV·m^2/kg. The stopping cross section $S(E)$ is thus given either by

$$S(E) \equiv -(1/N)\,(\mathrm{d}E/\mathrm{d}\lambda)$$

or by

$$S(E) \equiv -(1/\rho)\,(\mathrm{d}E/\mathrm{d}\lambda)$$

where $\mathrm{d}E/\mathrm{d}\lambda$ is the rate of loss of energy E with distance λ along the particle trajectory. Note that $\mathrm{d}E/\mathrm{d}\lambda$ is often called the stopping power although it is not in units of power.

Note 4 to entry: In some texts, the stopping cross section and stopping power are used interchangeably so that $S(E) \equiv -(\mathrm{d}E/\mathrm{d}\lambda)$. This inconsistency for the term stopping power leads to its deprecation.

Note 5 to entry: Older texts can be found with the stopping cross section given in keV·cm^2/gm (meaning “per gram”) and in many other forms.

4.12
electronic stopping cross section

<EIA, RBS, sputtering> *stopping cross section* (4.11) arising from energy transfer to the electrons of the sample

Note 1 to entry: The total stopping cross section is the sum of the electronic and *nuclear stopping cross sections* (4.13).

Note 2 to entry: The maximum of the nuclear stopping cross section occurs at energies of the order of 1 keV per nucleon, whereas that of the electronic stopping cross section occurs at above 100 keV per nucleon. The absolute value of the electronic stopping cross section maximum is significantly greater than that for the nuclear stopping cross section.

4.13
nuclear stopping cross section

<EIA, RBS, sputtering> *stopping cross section* (4.11) arising from energy transfer to atomic nuclei of the sample

Note 1 to entry: The total stopping cross section is the sum of the nuclear and *electronic stopping cross sections* (4.12).

Note 2 to entry: The maximum of the nuclear stopping cross section occurs at energies of the order of 1 keV per nucleon, whereas that of the electronic stopping cross section occurs at above 100 keV per nucleon. The absolute value of the electronic stopping cross section maximum is significantly greater than that for the nuclear stopping cross section.

4.14
Rutherford cross section

<RBS> *elastic scattering cross section* (4.8) calculated using classical mechanics and a Coulomb potential

Note 1 to entry: See *elastic scattering cross section* (4.8) and *enhanced elastic cross section* (4.21).

Note 2 to entry: The resulting cross section formula was first derived by Rutherford.

4.15
screening

response arising from the atom's electrons, causing an apparent reduction in the coulomb potential of the nucleus

Note 1 to entry: In *IBA* (17.1), when the incident ion is far from the target nucleus, the atom in which the nucleus sits looks neutral to the ion as a result of screening. The screening reduces the scattering *cross section* (4.7) slightly from the *Rutherford cross section* (4.14) (about 1 % per 50 increase in the target atomic number for 2 MeV He). The effect becomes more pronounced and increasingly uncertain as the energy decreases and, for *LEIS* (17.2), the cross section is no longer really well-known.

4.16
screening function

<IBA> factor by which the *Rutherford cross section* (4.14) is reduced as a result of *screening* (4.15) in a given situation

4.17
stopping power
stopping force

<EIA, RBS, sputtering> rate of *energy loss* (4.3) of a particle with distance along its trajectory in a sample

Note 1 to entry: See *stopping cross section* (4.11), *electronic stopping power* (4.18), and *nuclear stopping power* (4.19).

Note 2 to entry: Stopping power and stopping force are synonymous terms and are usually represented by $-\mathrm{d}E/\mathrm{d}\lambda$ for a particle of energy E moving along a path within a material.

Note 3 to entry: Stopping power is the official nomenclature of the International Commission on Radiation Units and Measurements (ICRU) but it is recognized that the term does not define a power but a force and so stopping force has been included here as a more precise synonymous term.

Note 4 to entry: In older texts, this quantity can also be called, erroneously, the stopping cross section.

4.18
electronic stopping power

contribution to the *stopping power* (4.17) due to interactions between the particle and electrons in the material

Note 1 to entry: see also *electronic stopping cross section* (4.12).

4.19
nuclear stopping power

contribution to the *stopping power* (4.17) due to interactions between the particle and atomic nuclei in the material

Note 1 to entry: see also *nuclear stopping cross section* (4.13).

4.20
Bragg's rule

empirical rule formulated by W.H. Bragg and R. Kleeman that states that the *stopping cross section* (4.11) of a compound sample is equal to the sum of the products of the elemental stopping cross sections for each constituent and its atomic fraction, that is,

$$S_{\mathrm{AB}}(\varepsilon)=xS_{\mathrm{A}}(\varepsilon)+yS_{\mathrm{B}}(\varepsilon)$$

where $S_{\mathrm{AB}}(\varepsilon)$ is the stopping cross section of the compound $\mathrm{A}_x\mathrm{B}_y$, and $S_{\mathrm{A}}(\varepsilon)$ and $S_{\mathrm{B}}(\varepsilon)$ are the stopping cross sections of elements A and B, respectively

4.21
enhanced elastic cross section

<ISS, RBS> *cross section* (4.7) of an atom for *elastic scattering* (4.1) that is greater than the *Rutherford cross section* (4.14) due to partial penetration of a nucleus in the sample by the incident particle

4.22
nuclear reaction cross section

<EIA> *cross section* (4.7) at a given *beam energy* (8.33) and emission direction of the detected product for a particular nuclear reaction per atom

Note 1 to entry: This cross section is usually expressed per atom as an area in units of barns (1 barn = 10^{-28} m^2).

4.23
resonance reaction

<EIA> nuclear reaction that has a narrow peak in the *nuclear reaction cross section* (4.22) as a function of energy, the nuclear reaction cross section at the peak being so much larger than the nuclear reaction cross sections at adjacent energies on either side of the peak that essentially all the particles detected from the reaction are due to the peak

4.24
Fano plot

plot of data for the non-relativistic *kinetic energy* (3.35), E, times a specified factor versus the logarithm of E to evaluate the consistency with, or divergence from, the rate of energy loss for a fast charged particle with distance described by Bethe's theory

Note 1 to entry: The plot is named after U Fano[6] who, based on the theory of Bethe,[7] proposed a plot for testing the number of ionizations per unit path, S, for a fast charged particle in a gas. In his relativistic approach, $2\beta^2S$ is plotted versus $\ln[\beta^2/(1-\beta^2)]-\beta^2$, where $\beta = v/c$, v being the particle velocity and c, the velocity of light. Fano plots have been utilized in analyses of sets of data for the electron *inelastic mean free path* (12.41), λ, in solid materials as a function of electron energy that were intended for use in *AES* (11.1) and XPS. In such applications, E/λ is plotted versus $\ln E$. In other applications, the product σE, where σ is the *cross section* (4.7) for a specified excitation or ionization, is plotted versus $\ln E$.

4.25
Barkas effect
Barkas-Andersen effect

deviation, for *heavy particles* (18.7), of the *electronic stopping cross section* (4.12) from that of the Bethe theory

Note 1 to entry: The Bethe theory is derived in Reference [7].

Note 2 to entry: Published effects occur in the energy range above 0,5 MeV.

4.26
ionization cross section

cross section (4.7) for a process that produces, in an atom, a vacancy in a previously occupied shell

Note 1 to entry: Total ionization cross section refers to removal of an electron from any atomic shell or sub-shell of the atom.

Note 2 to entry: Partial or sub-shell ionization cross section refers to removal of an electron from a specified shell or sub-shell of the atom.

Note 3 to entry: A partial ionization cross section can be expressed per electron in a shell or sub-shell or for the total number of these electrons in a shell or sub-shell of the particular atom.

Note 4 to entry: An atom can have multiple vacancies following an initial ionization or as the result of subsequent *Auger* (12.30) or *Coster-Kronig* (12.36) processes.

4.27
damage cross section

cross section (4.7) for the change in the number of particular entities considered to be a result of damage caused by bombardment by defined ions, electrons, or photons

Note 1 to entry: See *disappearance cross section* (20.16).

Note 2 to entry: The particular entities can, for example, be specific molecules on a *surface* (3.2), specific observed ion fragments, atoms in a given *chemical state* (12.23), or polymer cross-linking as inferred from spectral data.

Note 3 to entry: As a result of the break-up of larger entities, the observed entity can increase or decrease in intensity.

Note 4 to entry: Cross sections are often expressed as an area per target entity (atom, molecule, etc.) for the relevant process.

Note 5 to entry: Either as a result of the damage or as a result of electron or ion *sputtering* (9.3), the damaged material can be removed from the sample. For bulk samples, this can reduce any change in the relevant signal observed. For *monolayer* (5.6) samples, such sputtering can increase any change in the relevant signal observed. *Preferential sputtering* (9.26) can also change the relevant signal observed.

Note 6 to entry: A cross section of σ per atom for the removal of entities from a given state on a surface leads to a reduction dN in the number N of entities in that state in a time dt given by the relation:

$$\mathrm{d}N = -NJ\sigma\,\mathrm{d}t$$

where J is the primary-ion or electron *dose* (8.20) rate density.

Integration leads to the relation

$$N = N_0 \exp(-J\sigma t)$$

where N_0 is the initial value of N.

The observed value of the number of a given entity can also depend on sources creating that entity as discussed in Note 3 to entry.

4.28
attenuation coefficient

quantity μ in the expression $\mu\Delta x$ for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer Δx of a substance in the limit as Δx approaches zero, where Δx is measured in the direction of the beam

Note 1 to entry: See *attenuation length* (4.30) and *mass absorption coefficient* (4.39).

Note 2 to entry: The intensity or number of particles in the beam decays as $\exp(-\mu/x)$ with the distance x.

Note 3 to entry: The attenuation coefficient is the reciprocal of the attenuation length .

4.29
transport mean free path

λ_{tr}

average distance that an energetic particle travels before its momentum in its initial direction of motion is reduced to 1/e of its initial value by *elastic scattering* (4.1) alone

Note 1 to entry: See *inelastic mean free path* (12.41).

Note 2 to entry: For a homogeneous and isotropic solid, in which only binary elastic scattering occurs, the transport mean free path is related to the *transport cross section* (4.10), σ_{tr}, by

$$\lambda_{\mathrm{tr}} = \frac{1}{N\sigma_{\mathrm{tr}}}$$

where N is the number of scattering centres per unit volume.

4.30
attenuation length

quantity l in the expression $\Delta x/l$ for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer Δx of a substance in the limit as Δx approaches zero, where Δx is measured in the direction of the beam

Note 1 to entry: See *attenuation coefficient* (4.28), *decay length* (4.31), *effective attenuation length* (12.45), *electron inelastic mean free path* (12.41), and *mass absorption coefficient* (4.39).

Note 2 to entry: The intensity or number of particles in the beam decays as $\exp(-x/l)$ with the distance x.

Note 3 to entry: For electrons in solids, the behaviour only approximates to an exponential decay due to the effects of *elastic scattering* (4.1). Nevertheless, for some measurement conditions in *AES* (11.1) and *XPS* (11.6), the *signal intensity* (3.17) can depend approximately exponentially on path length, but the exponential constant (the parameter l) is normally different from the corresponding inelastic mean free path. Where that approximation is valid, the term effective attenuation length is used.

4.31
decay length

value of l for an intensity exhibiting a response $e^{\pm x/l}$ with distance x

Note 1 to entry: See *attenuation length* (4.30).

4.32
emission function decay length

negative reciprocal slope of the logarithm of the *emission depth distribution function* (4.35) at a specified depth

4.33
average emission function decay length

negative reciprocal slope of the logarithm of a specified exponential approximation to the *emission depth distribution function* (4.35) over a specified range of depths, as determined by a straight-line fit to the emission depth distribution function plotted on a logarithmic scale versus depth on a linear scale

4.34

deep emission function decay length

asymptotic value of the *emission function decay length* (4.32) for increasing depths from the *surface* (3.2)

4.35

emission depth distribution function

<for a measured signal of particles or radiation emitted from a surface> probability that the particle or radiation leaving the *surface* (3.2) in a specified state and in a given direction originated from a specified depth measured normally from the surface into the material

4.36

excitation depth distribution function

probability that specified excitations are created at specified depths measured, normally from a *surface* (3.2) into the material, by a beam of specified particles or radiation incident on the surface in a given direction

4.37

information depth

maximum depth, normal to the *surface* (3.2), from which useful information is obtained

Note 1 to entry: The information depths for the different surface analysis methods differ significantly. The information depth for each technique depends on the material being analysed, the particular signals being recorded from that material, and the instrument configuration.

Note 2 to entry: The information depth can be identified with the sample thickness from which a specified percentage (e.g. 95 % or 99 %) of the detected signal originates.

Note 3 to entry: The information depth can be determined from a measured, calculated, or estimated *emission depth distribution function* (4.35) for the signal of interest.

4.38

mean escape depth

average depth normal to the *surface* (3.2) from which the specified particles or radiations escape as defined by

$$\int_0^\infty z\phi(z,\theta)\,\mathrm{d}z \bigg/ \int_0^\infty \phi(z,\theta)\,\mathrm{d}z$$

where $\phi(z,\theta)$ is the *emission depth distribution function* (4.35) for depth z from the surface into the material and for *angle of emission* (8.5) θ with respect to the surface normal

4.39

mass absorption coefficient

mass attenuation coefficient

quantity μ/ρ in the expression, $(\mu/\rho)\Delta(\rho x)$, for the fraction of a parallel beam of specified particles or radiation removed in passing through a thin layer of mass thickness $\Delta(\rho x)$ of a substance in the limit as $\Delta(\rho x)$ approaches zero, where $\Delta(\rho x)$ is measured in the direction of the beam

Note 1 to entry: See *attenuation length* (4.30).

Note 2 to entry: The mass density of the substance is ρ, the reciprocal of the attenuation length is μ and x is the distance in the direction of the beam.

Note 3 to entry: The intensity or number of particles in the beam decays as $\exp(-\mu x)$ with the distance x.

Note 4 to entry: The mass attenuation (absorption) coefficient is the quotient of the *attenuation coefficient* (4.28) by the mass density of the substance.

4.40
Beer's law
Beer-Lambert law
law in which the signal of interest decays exponentially with distance travelled

Note 1 to entry: In electron spectroscopies, in the approximation in which the electrons are assumed to travel in straight lines, the electron intensity of interest decays with distance with a decay constant given by the *attenuation length* (4.30). In a more complete approach in which the *elastic scattering* (4.1) of the electrons is considered, the electron intensity of interest decays with distance along the no-longer straight trajectory with a decay constant given by the *inelastic mean free path* (12.41).

4.41
projected range
<EIA, RBS, SIMS> distance from the *surface* (3.2) at which an energetic ion or atom comes to rest in the sample, projected along the direction of the beam

Note 1 to entry: See *range straggling* (4.43).

Note 2 to entry: Calculations usually deal with the mean or average projected range for a large number of ions or atoms of the same species and the same energy.

4.42
transverse range
<EIA, RBS, SIMS> distance, normal to the direction of an energetic ion or atom impacting a *surface* (3.2), at which the ion or atom comes to rest in the sample

Note 1 to entry: See *projected range* (4.41).

4.43
range straggling
<EIA, RBS, SIMS> standard deviation of the *projected ranges* (4.41) of energetic ions or atoms of a given energy

Note 1 to entry: See *transverse straggling* (4.44).

4.44
transverse straggling
<EIA, RBS, SIMS> standard deviation of the *transverse ranges* (4.42) of energetic ions or atoms of a given energy

Note 1 to entry: See *range straggling* (4.43).

4.45
infratrack
region of a *primary ion* (20.26) track in an organic material up to 1 nm from the track centre

Note 1 to entry: See *ultratrack* (4.46).

Note 2 to entry: The energy deposited electronically is deposited mainly as primary excitations and ionizations in this region.

4.46
ultratrack
region of a *primary ion* (20.26) track in an organic material from 1 to 100 nm from the track centre

Note 1 to entry: See *infratrack* (4.45).

Note 2 to entry: The energy deposited electronically in this region is deposited mainly through *secondary electrons* (12.2) produced as a result of primary processes in the infratrack. For fast ions, this fraction of the energy deposition can exceed that in the infratrack.

4.47

radiation-enhanced diffusion

radiation-induced diffusion

atom movement in the solid, well beyond the typical penetration depth of an incident particle, due to particle beam damage or bombardment-induced defects

5 Terms related to the description of samples

5.1

reference material

RM

material, sufficiently homogeneous and stable with respect to one or more specified properties, which has been established to be fit for its intended use in a measurement process

[SOURCE: ISO Guide 30:1992+A1:2008[3]]

EXAMPLE Implanted silicon wafers to calibrate dopant levels; thin oxide layers on substrates to calibrate depth or thickness in analytical *depth profiling* (3.34) instruments.

Note 1 to entry: Some RMs involving surface properties can be in the form of wafers or foils. For these, the material is often homogeneous for the property values across the *surface* (3.2) but not in the direction perpendicular to the surface and into the bulk.

5.2

certified reference material

CRM

reference material (5.1) characterized by a metrologically valid procedure for one or more specified properties, accompanied by a certificate that provides the value of the specified property, its associated uncertainty, and a statement of metrological traceability

[SOURCE: ISO Guide 30:1992+A1:2008[3]]

Note 1 to entry: CRMs are usually prepared in batches for which the property values are determined within stated uncertainty limits by measurements on samples representative of the whole batch.

Note 2 to entry: All CRMs lie within the definition of "measurement standards" given in the international vocabulary of metrology, ISO/IEC Guide 99[6].

Note 3 to entry: Some *RMs* (5.1) and CRMs have properties which, because they cannot be correlated with an established chemical structure or for other reasons, cannot be determined by exactly defined physical and chemical measurement methods. Such materials include certain biological materials such as vaccines to which an international unit has been assigned by the World Health Organization.

5.3

interfacial region

volume between two bulk phases having chemical, elemental, or physical properties different from either bulk phase

5.4

segregation

partitioning of a species from one region to another as a result of kinetic or thermodynamic effects

Note 1 to entry: Segregation is often observed at *surfaces* (3.2) and *interfaces* (3.1).

5.5

surface segregation

partitioning of a species from the bulk of a material to the *surface* (3.2) as a result of kinetic or thermodynamic effects

5.6

monolayer

<chemisorption, physisorption, segregation> complete coverage of a substrate by one atomic or molecular layer of a species

5.7

monolayer capacity

<chemisorption> amount of adsorbate which is required to occupy all adsorption sites as determined by the structure of the adsorbent and by the chemical nature of the adsorptive

5.8

monolayer capacity

<physisorption> amount of adsorbate which is required to cover the *surface* (3.2) with a complete *monolayer* (5.6) of atoms or molecules in a close-packed array

Note 1 to entry: The type of close packing shall be stated.

5.9

surface coverage

<chemisorption, physisorption> quotient of the amount of a material at a *surface* (3.2) by a measure of the surface area

Note 1 to entry: The surface coverage can be expressed in atoms·m^{-2}, in mol·m^{-2}, in kg·m^{-2}, or as a ratio of the amount to the *monolayer capacity* (5.7) (5.8).

5.10

multilayer

structure composed of two or more chemically distinct layers

Note 1 to entry: See *delta layer* (5.12).

Note 2 to entry: This term is often applied to solid samples in which the layers are very uniform in thickness and for which the layer thicknesses are in the range 1 nm to 100 nm.

5.11

multilayer

<chemisorption, physisorption> coverage of a substrate surface by more than one atomic or molecular layer of the adsorptive or segregated species

Note 1 to entry: See *monolayer* (5.6).

5.12

delta layer

layer of discrete composition, one atom thick, formed during growth of material on a substrate

Note 1 to entry: These films are often formed during epitaxial growth on single-crystal substrates.

5.13

thin film

layer of material, typically less than 100 nm in thickness, deposited or grown on a substrate

Note 1 to entry: Films thinner than 10 nm are often called ultrathin films.

5.14

self-assembled monolayer

SAM

film, one molecule thick, covalently assembled on a *surface* (3.2)

5.15
Langmuir-Blodgett film
LB film
film comprising one or more *monolayers* (5.6) of organic molecules

Note 1 to entry: The films are transferred from the *surface* (3.2) of a liquid bath onto solid substrates and by repeated immersions many layers can be deposited. Control of the liquid surface tension during this process allows the molecular density of the monolayers to be controlled.

5.16
surface contamination
material, generally unwanted, on the sample *surface* (3.2) which either is not characteristic of that sample and any process investigated or has arisen from exposure of the sample to particular environments other than those relevant for the original surface or the process to be studied

Note 1 to entry: Common surface contaminants are hydrocarbons and water. Local reactions with these and the environment can lead to a wide range of oxidation and other products.

5.17
charge modification
alteration of the amount or the distribution of charge at a sample *surface* (3.2)

5.18
field-induced migration
effect occurring in insulators where internal electric fields created by ion or electron bombardment cause the migration of sample atoms

5.19
bond cleavage
bond scission
breakage of a molecular bond

Note 1 to entry: This breakage can lead to two fragments that can be charged or not charged, or to a single rearranged product.

Note 2 to entry: For α- and β-cleavage, see Reference [8] or [9].

5.20
surfactant
substance that lowers the interfacial energy of a material in contact with a liquid or the surface energy of that liquid

Note 1 to entry: In practice, the liquid is usually water or a water-based medium. Emulsifiers, detergents, and dispersing agents are examples of surfactants.

Note 2 to entry: In many cases, surfactant molecules have a hydrophilic or polar group at one end and a lipophilic or oleophilic group at the other.

5.21
tethering
process of attaching a molecule to a surface

Note 1 to entry: Molecules can be attached to surfaces by functionalizing the surface, or first adsorbing other *cross-linker* (5.22) molecules.

5.22
cross-linker
<adsorption> molecule with appropriate end groups to bond to both molecules adsorbed on a surface and further molecules which do not adsorb on those adsorbed molecules

5.23

polymer repeat unit

smallest structure that, repeated many times, describes the molecular structure of the polymer

5.24

dendrimer

molecule comprising a multifunctional core molecule with a dendritic wedge of highly branched monomers regularly attached to each functional site, leading to a monodisperse, tree-like, or generational structure

Note 1 to entry: Dendrimer synthesis occurs in polymer chemistry and involves stepwise reactions in which the dendrimer is built up one monomer layer, or generation, at a time. The core molecule is referred to as “generation 0”. Each successive *repeat unit* (5.23) along all branches forms the next generation, “generation 1”, “generation 2”, and so on until the terminating generation.

6 Terms related to sample preparation

6.1

cross-sectioning

sample preparation in which the sample is cleaved, cut, or polished in a plane perpendicular to the *interface* (3.1) under stuy, so that associated compositional differences or gradients can be observed in that plane

6.2

angle lapping

sample preparation in which a sample is mechanically polished at an angle to the original *surface* (3.2)

Note 1 to entry: See *ball catering* (6.3) and *radial sectioning* (6.4).

Note 2 to entry: This angle can often be less than 1° so that depth information with respect to the original surface is transformed to lateral information.

6.3

ball cratering

procedure in which the sample is abraded by a sphere in order to expose compositional changes in layers below the original *surface* (3.2) with the intent that the depth of those layers can be related to the lateral position in the crater created by the abrasion

Note 1 to entry: See *angle lapping* (6.2) and *radial sectioning* (6.4).

6.4

radial sectioning

sample preparation in which a sample is polished by a cylinder in order to expose compositional changes below the original sample *surface* (3.2) with the intent that the depth of these layers can be related to the position on the surface created by the cylinder

Note 1 to entry: See *angle lapping* (6.2) and *ball catering* (6.3).

6.5

spin coating

coating of a thin layer of an organic material deposited from solution, under the action of high-speed rotation, on a flat substrate wetted by that solution

Note 1 to entry: Rotation speeds of about 4 000 r/min are commonly used, producing films generally thinner than 100 nm.

Note 2 to entry: Some users place a drop of solution in the centre and some flood the whole sample, prior to the high-speed rotation that removes the solvent.

7 Terms related to instrumentation

7.1
synchrotron radiation
electromagnetic radiation (photons) with a continuous energy spectrum, created by the acceleration of electrons in a synchrotron or storage ring

7.2
instrumental background
intensity contribution, generally unwanted, arising from non-ideal behaviour of one or more parts of the instrument

7.3
internal scattering
process in which some particles strike internal *surfaces* (3.2) of the spectrometer in such a way that scattered or secondary particles are detected as unwanted intensity in the spectrum

7.4
solid angle of analyser
solid angle from a point on the sample that transmits particles or photons to the detector

Note 1 to entry: See *analyser transmission function* (7.15).

7.5
optical aperture
system consisting of a combination of a photon or particle lens and an aperture in an optical or particle spectrometer to limit the field of view for signal detection

7.6
selected-area aperture
<XPS, SIMS> aperture in the electron or ion optical system restricting the detected signal to a small area of the sample *surface* (3.2)

Note 1 to entry: See *optical aperture* (7.5).

7.7
contrast aperture
aperture, in an ion or electron optical system, designed to reduce unwanted *background signal* (3.21)

Note 1 to entry: This aperture can also govern the *spatial resolution* (10.14) and other properties of the system.

7.8
detector efficiency
fraction of particles or photons incident on the detector that result in the detected signal

7.9
instrumental detection efficiency
ratio of the quantity of a detected event to the quantity of that event available for measurement

7.10
spectrometer dispersion
analyser dispersion
<energy or mass> quotient of the change in position, Δx, of the dispersed particles at the exit of an analyser or a spectrometer by the fractional change in particle energy, $\Delta E/E$, or mass, $\Delta m/m$

7.11
spectrometer dispersion
analyser dispersion
<optical> quotient of the change in position, Δx, of the radiation at the exit of the spectrometer by the change in wavelength, $\Delta \lambda$

7.12
spectrometer étendue

integral of the product of the spectrometer transmission and an element of area of a plane *surface* (3.2), normal to the analyser axis passing through the centre of the *analysis area* (8.49), over that surface

Note 1 to entry: The units of étendue can be sr·m^2·eV, sr·m^2·amu, or sr·m^3.

7.13
spectrometer response function

quotient of the number of particles detected with a spectrometer by the number of such particles per solid angle and per interval of the dispersing parameter available for measurement as a function of the dispersing parameter

Note 1 to entry: See *spectrometer étendue* (7.12).

Note 2 to entry: The dispersing parameter is commonly energy, mass, or wavelength.

Note 3 to entry: The units of the spectrometer response function can be sr·eV, sr·amu, or sr·m.

Note 4 to entry: The spectrometer response function is similar to the *spectrometer transmission function* (7.15) or étendue but includes the efficiencies of all other components of the measurement chain, such as detectors and the electronic processing and recording equipment.

Note 5 to entry: For some methods of *quantitative analysis* (3.8), the energy dependence of the response function is required in order to use *relative sensitivity factors* (12.91). For these cases, a function is determined which is proportional to the absolute response function, where the proportionality constant is not necessarily important.

7.14
relative instrument spectral response function
RISR

<AES, SIMS, XPS> ratio of the *spectrometer response function* (7.13) to the response function of a reference instrument, or the average for several such instruments, as a function of energy [*AES* (11.1), *XPS* (11.6), etc.] or mass (*SIMS* (19.1))

Note 1 to entry: The RISR can be used to relate spectra from one instrument to spectra from another when using similar excitation sources and geometries.

7.15
spectrometer transmission function
analyser transmission function

quotient of the number of particles transmitted by the analyser by the number of such particles per solid angle and per interval of the dispersing parameter (e.g. energy, mass, or wavelength) available for measurement as a function of the dispersing parameter

Note 1 to entry: See *spectrometer response function* (7.13).

Note 2 to entry: The units of transmission can be sr·eV, sr·amu, or sr·m.

Note 3 to entry: Often, an incomplete use of the term occurs where just the solid angle of acceptance of the spectrometer, in sr, or a fraction of the 2π solid angle of available space is given. This usage is deprecated, cf. *solid angle of analyser* (7.4).

Note 4 to entry: This term is often used incorrectly instead of spectrometer response function, which includes contributions from the detector and the signal-processing system.

7.16
Faraday cup
detector with a cup-shaped electrode for collection of the electric charge carried by a beam of charged particles passing into the cup, designed such that emission of charged particles from the detector is minimized

Note 1 to entry: A Faraday cup is of "black hole" quality if it is open only to charged particles moving from outside in, but not to charged particles of any type moving from inside out. As a detector for ions in a beam, a Faraday cup is "ideal" if it combines a black-hole capability with a filter for electrons and *secondary ions* (20.28) (i.e. the Faraday cup is open only to forward-moving ions of the beam, but is closed to all electrons and secondary ions from both inside and outside the cup).

7.17
dead time
time per pulse for which a pulse-counting system is unavailable for further counting

7.18
non-extended dead time
dead time (7.17) for a system where the pulse lengths are not extended by extra pulses arriving during the dead time associated with earlier pulses

7.19
extended dead time
dead time (7.17) for a system where the pulse lengths are extended by extra pulses arriving during the dead time associated with an earlier pulse

7.20
multidetector dead time
effective *dead time* (7.17) of the whole detector, treating it as a single detector

7.21
post-acceleration detector voltage
post-acceleration voltage
voltage applied to the front of the detector to increase the *impact energy* (8.35) of incident electrons or ions

Note 1 to entry: Voltages are often referred to reference points in the instrumental electronics, but here the reference zero is such that a post-acceleration detector voltage of 5 kV leads to an impact energy of 5 keV, etc. Post-acceleration detector voltages of 5 kV to 20 kV are generally used.

7.22
beam blanking
electrostatic or electromagnetic process designed to prevent *beam particles* (8.9) from impacting the sample when activated

Note 1 to entry: See *beam bunching* (20.44) and *beam chopper* (20.48).

Note 2 to entry: For pulsed *ion beams* (8.8), the beam is usually deflected into a beam collector from which no particles can reach the sample and where the process of *sputtering* (9.3) causes minimal effect on nearby components of the ion optical system.

7.23
chromatic aberration
non-ideal focus of an particle optical system for particles of different energies

7.24
energy acceptance window
range of energies accepted by a spectrometer, leading to a detected signal

7.25
dynamic emittance matching

electron or ion optical method of steering a spectrometer axis to align with the impact area of the *primary beam* (8.10) at all points of a *raster* (8.38) scan on the sample *surface* (3.2)

7.26
FIB

focussed ion beam system

ion beam (8.8) system used for machining small regions with sub-micron precision

Note 1 to entry: FIB-machined *surfaces* (3.2) can have an ion-damaged surface that requires removal.

7.27
gas cluster ion beam

GCIB

ion beam (8.8) formed of *cluster ions* (3.44) by ionising condensed clusters of atoms or molecules that are gaseous at ambient temperature and pressure

7.28
liquid-metal ion gun

LMIG

ion gun utilizing a liquid-metal Taylor cone as the source of the *primary ions* (20.26)

Note 1 to entry: The Taylor cone generates ion sources of very high brightness. This design enables the gun to provide *beam diameters* (8.30) in the range 50 nm to 1 µm for ion *beam energies* (8.33) in the range 5 keV to 30 keV, the lowest diameters generally being at the higher energies.

7.29
intrinsic linewidth

<instrument> see *resolution of a spectrometer* (10.6)

7.30
raw-data file

unprocessed-data file of information provided by an instrument

Note 1 to entry: For *time of flight* (20.49) SIMS instruments, this file usually contains the *x*- and *y*-coordinates of the *ion beam* (8.8) *raster* (8.38) address as well as the recorded flight times and signal intensities since these files are used retrospectively to generate secondary-ion *maps* (8.57) or spectra from the whole or selected parts of the map, or to generate these from all or selected time regions.

8 Terms related to experimental conditions

8.1
angle of incidence

incidence angle

angle between the incident beam and the local or average surface normal

Note 1 to entry: The particular surface normal, such as the surface normal to an elementary portion of a rough *surface* (3.2) or the normal to the average surface plane, shall be specified.

8.2
glancing angle

grazing angle

angle between the incident beam and the average surface plane

Note 1 to entry: The *angle of incidence* (8.1) and the glancing angle are complementary.

8.3
grazing incidence
glancing incidence
geometrical arrangement in which the angle of the incident particles or photons is near 90° from the normal to the sample *surface* (3.2)

Note 1 to entry: This configuration can result in improved surface sensitivity.

8.4
angle of scattering
scattering angle
angle between the direction of the incident particle or photon and the direction that the particle or photon is travelling after scattering

8.5
angle of emission
emission angle
angle between the trajectory of a particle or photon as it leaves a *surface* (3.2), and the local or average surface normal

Note 1 to entry: The particular surface normal shall be specified.

Note 2 to entry: The angle of emission is the complement of the *take-off angle* (8.7).

8.6
grazing exit
glancing exit
geometrical arrangement in which the angle of the scattered (or emitted) particles or photons is near 90° from the normal to the sample *surface* (3.2)

Note 1 to entry: This configuration generally results in improved surface sensitivity and can also improve *depth resolution* (10.18).

8.7
take-off angle
angle between the trajectory of a particle as it leaves a *surface* (3.2) and the local or average surface plane

Note 1 to entry: The particular surface plane shall be specified.

Note 2 to entry: The take-off angle is the complement of the *angle of emission* (8.5).

Note 3 to entry: In the past, take-off angle has sometimes been used erroneously to mean angle of emission.

8.8
ion beam
directed *flux* (8.18) of charged atoms or molecules

8.9
beam particle
electron, positron, ion, atomic, molecular, or cluster species contained in the incident beam

8.10
primary beam
directed *flux* (8.18) of particles or photons incident on a sample

8.11

beam current

I

quotient of dQ by dt, where dQ is the quantity of electric charge of a specified polarity in the beam passing in the time interval dt

$$I = \mathrm{d}Q/\mathrm{d}t$$

Note 1 to entry: See *pulse beam current* (8.15) and *average beam current* (8.12).

Note 2 to entry: For beams in which the current varies with time, the instantaneous and time-averaged beam currents generally differ. For a pulsed beam, the current when the beam is on can be equal or not equal to the DC, or unpulsed, beam current.

8.12

average beam current

quotient of Q by t, where Q is the quantity of electric charge of a specified polarity in the beam passing in the time interval t

Note 1 to entry: For beams in which the instantaneous current varies periodically with time, the time interval t is an integral number of periods.

8.13

beam current density

J

<for a parallel beam of charged particles> quotient of dI by dA, where dI is the element of *beam current* (8.11) incident on an area dA at right angles to the direction of the beam

$$J = \mathrm{d}I/\mathrm{d}A$$

Note 1 to entry: See *fluence* (8.16), *flux* (8.18), and *dose* (8.20).

Note 2 to entry: For a convergent or divergent beam, the area dA is replaced by a small sphere of cross-sectional area dA.

8.14

integrated beam current

total electric charge transported in the beam over a specified time

8.15

pulse beam current

quotient of Q by t_p where Q is the quantity of electric charge of a specified polarity in the beam passing during the period t_p in which the pulse is on

8.16

fluence

F

<for a parallel beam of particles> quotient of dN by dA, where dN is the number of particles of a specified type incident on an area dA at right angles to the direction of the beam:

$$F = \mathrm{d}N/\mathrm{d}A$$

Note 1 to entry: For a scanned parallel beam, the fluence can be referred to the laboratory coordinate system or to the scanned beam's own moving coordinate system. The latter generally gives the higher value. The usage of fluence in these situations requires a clear statement of the coordinate system being used.

Note 2 to entry: In some texts, the term fluence is used for *areic dose* (8.20). This is incorrect and has led to confusion. See Note 2 to entry in 8.20.

Note 3 to entry: See also *flux density* (8.19).

8.17

fluence

F

<for particles moving in many directions> quotient of dN by dA, where dN is the number of particles of a specified type incident on a sphere of cross-sectional area dA

8.18

flux

Φ

<for a beam of particles> quotient of dN by dt, where dN is the number of particles of a specified type passing in the time interval dt

$$\Phi = \mathrm{d}N/\mathrm{d}t$$

Note 1 to entry: See also *flux density* (8.19).

8.19

flux density

fluence rate

<for a beam of particles> quotient of dN by dt and dA, where dN is the number of particles of a specified type incident on a sphere of cross-sectional area dA passing in the time interval dt

8.20

areic dose

dose

D

quotient of dN by dA, where dN is the number of energetic particles of a specified type introduced into a solid through a surface area dA:

$$D = \mathrm{d}N/\mathrm{d}A$$

Note 1 to entry: The energetic particles are atoms or atom clusters, which can be electrically charged or neutral, and the surface area dA is the geometric surface area.

Note 2 to entry: For a stationary parallel beam, the areic dose equals the *fluence* (8.16) times cosθ, where θ is the *angle of incidence* (8.1) of the beam to the surface normal.

Note 3 to entry: In some texts, the term dose density is used, but the term dose more correctly areic dose) is more widespread. The term dose has been defined very differently in the fields of radiation and the medical sciences. The total quantity of particle radiation impacting the *surface* (3.2) has been taken by some to be dose, and the quotient of the quantity by the area of the surface to be dose by others. Here, dose is taken to be the latter. Dose density and dose, where they occur, are to be understood as the areic dose.

Note 4 to entry: For a discussion of areic dose in relation to ion-implanted *reference materials* (5.1), see Reference [10].

8.21

areic dose rate

G

quotient of dD by dt, where dD is the *areic dose* (8.20) introduced into a solid in time interval dt:

$$G = \mathrm{d}D/\mathrm{d}t$$

Note 1 to entry: For a stationary parallel beam, the areic dose rate equals the *flux* (8.18) times cosθ, where θ is the *angle of incidence* (8.1) of the beam.

8.22
implanted areic dose

D_{imp}

quotient of $\mathrm{d}N_{\text{imp}}$ by $\mathrm{d}A$, where $\mathrm{d}N_{\text{imp}}$ is the number of energetic particles of a specified type incident on a solid within a surface area $\mathrm{d}A$ and stopped within the solid:

$$D_{\text{imp}} = \mathrm{d}N_{\text{imp}} / \mathrm{d}A$$

Note 1 to entry: Particles which are not stopped within the solid are either backscattered or transmitted.

8.23
nominal areic dose

D_{nom}

areic dose (8.20), as measured by an approximating procedure

Note 1 to entry: Typically, D_{nom} for a beam of charged particles is derived by forming the quotient of the particle equivalent of the current integral over time and the surface area over which the beam is scanned with lateral uniformity. Hence, D_{nom} is generally an approximate average measure of D.

8.24
non-implanted areic dose

areic dose (8.20) representing the fraction of the *received areic dose* (8.25) not trapped in the sample

Note 1 to entry: The sum of the *implanted areic dose* (8.22) and the non-implanted areic dose equals the received areic dose.

8.25
received areic dose

D_{rec}

quotient of $\mathrm{d}N_{\text{rec}}$ by $\mathrm{d}A$, where $\mathrm{d}N_{\text{rec}}$ is the number of energetic particles of a specified type incident on a solid within a surface area $\mathrm{d}A$:

$$D_{\text{rec}} = \mathrm{d}N_{\text{rec}} / \mathrm{d}A$$

8.26
retained areic dose

D_{ret}

quotient of $\mathrm{d}N_{\text{ret}}$ by $\mathrm{d}A$, where $\mathrm{d}N_{\text{ret}}$ is the number of energetic particles of a specified type incident on a solid within a surface area $\mathrm{d}A$ which are stopped within the solid and remain therein:

$$D_{\text{ret}} = \mathrm{d}N_{\text{ret}} / \mathrm{d}A$$

Note 1 to entry: Particles which are stopped within the solid but do not remain therein can be either thermally evaporated or re-emitted by sputter erosion of the solid.

Note 2 to entry: The retained areic dose is a fractional quantity of the *implanted areic dose* (8.22).

8.27
sputtered areic dose

areic dose (8.20) representing the fraction of the *implanted areic dose* (8.22) lost from the sample by *sputtering* (9.3)

Note 1 to entry: The sputtered areic dose is a fractional quantity of the implanted areic dose.

8.28
damage limit

particle *areic dose* (8.20) above which significant changes in the spectrum or in a stated peak, arising from damage processes, are observed

Note 1 to entry: See *static limit* (20.57).

8.29

beam profile

spatial distribution of the beam *flux* (8.18) in a plane normal to the beam axis

8.30

beam diameter

<for a particle beam of circular cross section> full width of the beam at half maximum *flux density* (8.19)

Note 1 to entry: The beam diameter is usually specified at a given point in space, such as the position of the sample.

8.31

beam divergence angle

angular interval containing all or a specified fraction of the beam in the space after the focal plane

Note 1 to entry: See *beam convergence angle* (8.32).

Note 2 to entry: Where the beam is symmetrical, the full or semi-angle can be used. The particular measure of angle shall be stated.

8.32

beam convergence angle

angular interval containing all or a specified fraction of the beam in the space prior to or at the focal plane

Note 1 to entry: See *beam divergence angle* (8.31).

Note 2 to entry: Where the beam is symmetrical, the full or semi-angle can be used. The particular measure of angle shall be stated.

8.33

beam energy

kinetic energy (3.35) of the *beam particles* (8.9)

Note 1 to entry: See *impact energy* (8.35) and *incident particle energy* (8.34).

Note 2 to entry: The energy is usually given in electron volts.

Note 3 to entry: The beam energy is often taken to be the particle energy on impact at the sample *surface* (3.2). However, where a sample is at a potential other than ground, the impact energy of the particles can differ from the beam energy as delivered by an electron or ion gun to the sample environment. In this case, use of the term impact energy avoids confusion.

8.34

incident particle energy

kinetic energy (3.35) of a particle incident on the sample *surface* (3.2)

Note 1 to entry: See *beam energy* (8.33) and *impact energy* (8.35).

Note 2 to entry: The incident energy can also be expressed per atom for an incident atomic cluster; however, to avoid confusion, the phrase “per atom” should then be used.

8.35

impact energy

kinetic energy (3.35) of the particles on impact with the sample *surface* (3.2)

Note 1 to entry: See *beam energy* (8.33) and *incident particle energy* (8.34).

Note 2 to entry: For *primary-ion beams* (8.10) in *SIMS* (19.1), the ion impact energy is given by the difference in electric potential between the ion source and the sample surface multiplied by the charge on the ion.

Note 3 to entry: Use of the qualifier “impact” indicates that this is the energy of the particles striking the surface.

8.36

impact energy per ion

kinetic energy (3.35) of the *beam particles* (8.9) on impact

Note 1 to entry: See *impact energy* (8.35).

8.37

ion implantation

injection of ions into a sample

8.38

raster

two-dimensional pattern generated by the deflection of a *primary beam* (8.10)

Note 1 to entry: Commonly used rasters cover square or rectangular areas.

8.39

random raster

digital *raster* (8.38) array in which the coordinates of sequential ion pulses filling a frame are random

Note 1 to entry: The coordinates can be addressed in the same “random” sequence in each frame.

Note 2 to entry: A random raster, as opposed to a traditional or saw-tooth raster, can be used for analysing insulating samples to reduce the instantaneous accumulation of charge in any local region.

8.40

energy per channel

energy difference between successive spectral channels

8.41

sample bias

potential applied to the whole or part of the sample, referenced to the potential of the sample holder

Note 1 to entry: See *sample voltage* (8.43).

8.42

sample charging

change in the electrical potential in the sample or on the sample *surface* (3.2) caused by particle or photon bombardment

8.43

sample voltage

voltage of the sample referenced to ground

Note 1 to entry: See *sample bias* (8.41).

Note 2 to entry: The sample voltage can be pulsed or constant, depending on the type of instrument.

Note 3 to entry: For insulators, the sample voltage is assumed to be the same as that of the sample holder if an effective *charge neutralizing* (8.45) device is used.

8.44

charging potential

electrical potential of the surface region of an insulating sample, caused by irradiation

Note 1 to entry: Different charging potentials can occur on different areas or at different depths in a sample, arising from sample inhomogeneities or non-uniform intensity of the incident *flux* (8.18) of radiation.

Note 2 to entry: The surface and bulk potentials can differ, for example as a result of band bending, *interface* (3.1) dipoles and charge centres.

8.45

charge neutralization

maintenance at a fixed potential, usually near neutrality, of the *surface* (3.2) of a non-conducting or poorly conducting sample material under bombardment by primary particles or photons

Note 1 to entry: Charge neutralization can be accomplished by bombarding the surface with electrons or, more rarely, ions or photons.

8.46

electron flooding

irradiation of a sample with low-energy electrons in order to change or stabilize the *charging potential* (8.44)

8.47

analysis volume

<spectrometer> three-dimensional region within the spectrometer from which the entire analytical signal or a specified percentage of that signal can be detected

8.48

analysis volume

<sample> three-dimensional region of a sample from which the entire analysis signal or a specified percentage of that signal is detected

8.49

analysis area

<spectrometer> two-dimensional region of a sample *surface* (3.2) at the analytical point but set in the plane at right angles to the spectrometer axis from which the entire analytical signal or a specified percentage of that signal is detected

8.50

information area

area of a region in the plane of the *surface* (3.2) from which useful information is obtained

Note 1 to entry: The information area can be identified with the minimum surface area from which a specified percentage (e.g. 95 % or 99 %) of the detected signal originates.

Note 2 to entry: The information area can be determined from a measured, calculated, or estimated measure of the *signal intensity* (3.17) as a function of position on the sample surface.

8.51

information radius

maximum radius of a circular region, in the plane of the *surface* (3.2), from which useful information is obtained

Note 1 to entry: This definition is useful only for surface analyses of a homogeneous sample and for either normal incidence of the *primary beam* (8.10) or normal detection of the signal particles, in which it is expected that the *signal intensity* (3.17) as a function of position on the surface depends only on the radial distance from the axis of symmetry. If these conditions are not met, it is more appropriate to make use of the *information area* (8.50).

Note 2 to entry: The information radius can be identified with the radius within which a specified percentage (e.g. 95 % or 99 %) of the detected signal originates.

Note 3 to entry: The information radius can be determined from a measured, calculated, or estimated measure of the signal intensity as a function of radius.

8.52

sample area viewed by the analyser

two-dimensional region of a sample *surface* (3.2), measured in the plane of that surface, from which the analyser can collect an analytical signal from the sample or a specified percentage of that signal

8.53

gated area

defined area within a larger area from which the signal can be obtained

Note 1 to entry: The defined area is often in the central region of a crater and can be defined by an *optical aperture* (7.5), an *electronic gate* (8.55) or a *digital gate* (8.54).

8.54

digital gate

system allowing the data associated with any selected group of *map* (8.57) pixels to be summed to produce cumulative data from any desired area

8.55

electronic gate

system consisting of a counter or detector which is enabled or disabled by signals from the beam scanning system so that *counts* (3.18) only accumulate when the *primary beam* (8.10) is incident on a selected part of the mapped area

8.56

line scan

plot of the output *signal intensity* (3.17) from the spectrometer, the signal intensity from another detector, or processed intensity information from the available software along a line corresponding to a line on the sample *surface* (3.2)

Note 1 to entry: The line is most often an *x*- or *y*-linescan from a rectangular *raster* (8.38) but, in more sophisticated systems, may be in any arbitrary direction.

8.57

map

two- or three-dimensional representation of the sample *surface* (3.2) where the information at each point in the representation, given by a brightness or colour or as a length in a third dimension, is related to the output signal from a detector or processed intensity information from the available software

Note 1 to entry: By convention, the term image is usually applied to cases where the information is primarily optical. An exception is the term *ion image* (20.63) used in mass spectrometry.

Note 2 to entry: Maps are usually formed either by using a rectangular *raster* (8.38) of the *primary beam* (8.10) or by using an imaging detection system.

Note 3 to entry: Map intensities can be presented in a normalized fashion to have the maximum and minimum signal intensities set at, for example, full white and full black, respectively, or on a colour scale. The contrast scale should be defined.

8.58

chemical map

map (8.57) using signals proportional to the quantity of an element in a particular *chemical state* (12.23) in the sample

8.59

elemental map

map (8.57) using signals proportional to the quantity of an element present in the sample

8.60

topographic contrast

contrast in a *map* (8.57) or *ion image* (20.63) arising from the topography of the sample *surface* (3.2)

Note 1 to entry: Topographic effects can modify the interaction between the *primary beam* (8.10) and the sample, making the interpretation of electron or ion yield data more complex than otherwise.

Note 2 to entry: Topographic contrast can change after ion *sputtering* (9.3).

9 Terms related to sputter depth profiling

9.1
sputter depth profile
SDP
compositional depth profile (3.33) obtained when the surface composition is measured as material is removed by *sputtering* (9.3)

Note 1 to entry: In some analytical methods such as *SIMS* (19.1), the sputtering is often accomplished by the *ion beam* (8.8) used for analysis, but in other methods an ion beam is required.

9.2
ultra-shallow depth profile
<SIMS> *depth profile* (3.32) for which the depth over which significant changes occur is less than 10 nm

9.3
sputtering
process in which atoms and ions are ejected from the sample as a result of particle bombardment

9.4
collision cascade
sequential energy transfer between atoms in a solid as a result of bombardment by an energetic species

Note 1 to entry: See *atomic mixing* (9.9), *cascade mixing* (9.11), and *knock-on* (9.12).

9.5
linear cascade
linear collision cascade
dilute *collision cascade* (9.4) in which the number of atoms set in motion by an energetic primary particle is proportional to the amount of recoil energy deposited in the material

Note 1 to entry: See *spike* (9.6) and *thermal spike* (9.7).

Note 2 to entry: The *sputtering* (9.3) of solids by monatomic *primary ions* (20.26) in the energy range below 20 keV, usually used for surface analysis, is often assumed to be described by a linear collision cascade.

9.6
spike
<SIMS, sputtering> limited region in space and time within which the majority of atoms in an irradiated material are in rapid motion

Note 1 to entry: See *thermal spike* (9.7).

Note 2 to entry: The term spike is usually applied to the region generated by a single primary particle. In *SIMS* (19.1), this primary particle can often be a *cluster ion* (3.44).

9.7
thermal spike
<SIMS, sputtering> *spike* (9.6) in which energy deposition leading to local heating is the dominating process

Note 1 to entry: Other processes proposed to generate spikes are pressure and shock waves.

9.8
ion beam induced mass transport
movement of atoms in a sample caused by ion bombardment

9.9
atomic mixing
migration of sample atoms due to energy transferred into the surface region from incident particles

Note 1 to entry: See *cascade mixing* (9.11), *collision cascade* (9.4), and *knock-on* (9.12).

9.10
zone of mixing

layer of the sample *surface* (3.2) within which the *primary beam* (8.10) causes *atomic mixing* (9.9)

Note 1 to entry: See *collision cascade* (9.4).

9.11
cascade mixing

diffusion-like process in which atoms of material are moved randomly by energy deposited by incident particles slowing down in the sample surface region

Note 1 to entry: See *atomic mixing* (9.9), *collision cascade* (9.4) and *knock-on* (9.12).

Note 2 to entry: If atomic mixing and knock-on effects are not significant, the measured *sputter depth profile* (9.1) of a *delta layer* (5.12) is asymmetric on account of cascade mixing since the *surface* (3.2) moves through the sample as it is sputtered. The initial internal profile produced is Gaussian, however, until significant delta material has been lost through the sample surface.

Note 3 to entry: If cascade mixing is the only significant mixing process, the centroid of the measured distribution lies at the true delta position (after any shift in the depth scale arising from pre-equilibrium effects has been corrected).

Note 4 to entry: In the *dilute limit* (20.15), the measured *depth profile* (3.32) for the delta layer has an exponential tail because any internal atom has an equal probability of being moved deeper or shallower and there is thus an indefinitely persistent but decaying concentration in the near-surface region. The presence of this tail often leads to the belief that there is a directional knock-on process at work. True knock-on effects have rarely if ever been observed, however, and are probably not significant as causes of sputter profile distortion.

9.12
knock-in
knock-on
recoil implantation

movement of constituent atoms of the sample deeper into the sample as a result of collisions with a primary particle

Note 1 to entry: See *atomic mixing* (9.9), *cascade mixing* (9.11), and *collision cascade* (9.4).

Note 2 to entry: The knock-in process refers only to the forward movement of the constituent atoms (in the direction of the primary bombardment) whereas cascade mixing refers, in addition, to the backward movement of these atoms.

9.13
collective motion

<SIMS, sputtering> movement of a number of atoms or molecules at the same time and in the same region

9.14
leading edge decay length

value of the *decay length* (4.31) for an increasing *signal intensity* (3.17) as a function of depth prior to a maximum

Note 1 to entry: This term is mainly used in the SIMS *depth profiling* (3.34) of *delta layers* (5.12). It is also used in *AES* (11.1) and XPS *sputter depth profiles* (9.1).

9.15
trailing edge decay length

value of the *decay length* (4.31) for a decreasing *signal intensity* (3.17) as a function of depth following a maximum

Note 1 to entry: This term is mainly used in the SIMS *depth profiling* (3.34) of *delta layers* (5.12). It is also used in *AES* (11.1) and XPS *sputter depth profiles* (9.1).

9.16
cooperative uplifting

collective motion (9.13) of atoms or molecules under an atom or molecule at a *surface* (3.2), causing its desorption

9.17
altered layer

<particle bombardment> surface region of a material under particle bombardment where the *chemical state* (12.23) or physical structure is modified by the effects of the bombardment

Note 1 to entry: The *depth resolution* (10.18) in *SIMS* (19.1) can be greater or smaller than the altered-layer thickness, depending on the *analyte* (3.4) and bombarding-*ion species* (3.36).

9.18
erosion rate

<surface> quotient of the change in the position of the *surface* (3.2) as a result of particle or photon irradiation by the time of irradiation

Note 1 to entry: See *sputtering rate* (9.19).

Note 2 to entry: The erosion rate can be deduced from surface profilometer measurements of a crater after analysis. In this case, the effects of the *altered layer* (9.17) and post-profile oxidation can affect the measurement.

Note 3 to entry: Where the erosion is caused by *sputtering* (9.3), initially the erosion rate can be less than the sputtering rate as a result of the retention of sputtering particles.

Note 4 to entry: The rate can be measured as a velocity.

9.19
sputtering rate

quotient of the amount of sample material removed, as a result of particle bombardment, by time

Note 1 to entry: See *erosion rate* (9.18).

Note 2 to entry: The rate can be measured as a velocity, a mass per unit area per unit time, or some other measure of quantity per unit time.

9.20
relative sputtering rate

quotient of the *sputtering rate* (9.19) of a sample and the sputtering rate of a reference sample sputtered under the same conditions

9.21
crater depth

average depth of the region of a crater from which the measured signal is derived

Note 1 to entry: The crater is generally formed by ion bombardment in *sputter depth profiling* (9.1) and, in this case, can be different from the thickness of sample material removed by *sputtering* (9.3) due to dilation of the *altered layer* (9.17).

Note 2 to entry: The crater depth can be modified by the formation of a reacted layer (e.g. an oxide) following any exposure to the atmosphere or other environments necessary when conducting the crater depth measurement.

9.22
crater edge effect

occurrence of signals from the crater edge which often originate from depths shallower than the central region of the crater formed in *sputter depth profiling* (9.1)

9.23
volume yield

ratio of the total volume sputtered from a sample to the total number of incident particles

Note 1 to entry: See *fractional ion yield* (20.13), *fractional sputtering yield* (20.5), *negative-ion yield* (20.10), *partial ion yield* (20.12), *partial sputtering yield* (20.6), and *positive-ion yield* (20.11).

Note 2 to entry: The volume yield is useful for expressing the amount sputtered in organic layers where molecules can be easily fragmented and values of the molecular *sputtering yield* (20.4) can be much more variable between samples than the volume yield.

9.24
enhancement factor

$K_{n,1}$

<SIMS, sputtering> ratio of the ion or neutral *sputtering yield* (20.4) using a primary-ion cluster of n similar atoms to n times the ion or neutral sputtering yield using a *primary ion* (20.26) of one of those atoms where the primary-ion energy per atom is the same in each case

Note 1 to entry: An enhancement factor greater than unity in *SIMS* (19.1) is usually used to show that the yield from a cluster source is greater than the yield that would be predicted for a *linear collision cascade* (9.5).

9.25
equilibrium surface composition sputtering

steady state surface composition produced by *sputtering* (9.3) a homogeneous sample under non-varying conditions

9.26
preferential sputtering

change in the equilibrium surface composition of the sample which can occur when *sputtering* (9.3) multicomponent samples

9.27
steady state sputtering

<AES, GDS, SIMS> state of the *sputtering* (9.3) process in which important operational and analytical parameters are unchanging over a meaningful timescale

Note 1 to entry: See *stoichiometric sputtering* (9.28).

Note 2 to entry: Generally, steady state and stoichiometric sputtering are equivalent but, in profiling dilute *delta layers* (5.12) in semiconductors, for example, the sputtering can be at a steady state while the constituents being studied are not being sputtered in their stoichiometric ratio.

9.28
stoichiometric sputtering

<AES, GDS, SIMS> state of the *sputtering* (9.3) process in which the relative amounts of the elemental components sputtered from a sample are equal to their stoichiometry within the sample

Note 1 to entry: See *steady state sputtering* (9.27).

Note 2 to entry: For most homogeneous materials, stoichiometric sputtering is attained after the sputter removal of a few nanometres from the surface.

9.29
redeposition

deposition of sputtered sample material back onto the sample *surface* (3.2)

10 Terms related to resolution

10.1
resolution

quantity which describes the minimum distinguishable separation between features or regions in *measurand* (3.3) space

Note 1 to entry: In practice, many different resolution criteria are used. The choice depends on the measurand, the circumstances and the required use of the measure.

Note 2 to entry: Where necessary, resolution should be specified by the input measurand or resolution criterion as adjectives. For example, *energy resolution* (10.24) specifies energy as the input measurand and *FWHM resolution* (10.9) or *X% peak width resolution* (10.10) defines the resolution criterion. If both require specification it is recommended that the resolution criterion is listed first, e.g. ‘FWHM energy resolution’ and ‘12/88 depth resolution’.

Note 3 to entry: Resolution has the same dimensions as the measurand.

10.2
resolution function

normalised output signal distribution as a function of variable input *measurand* (3.3) values which arises from a feature with a single measurand value

Note 1 to entry: For direct measurement of a resolution function the feature should be much smaller than the width of the resolution function. If the feature is larger than the width of the resolution function, but has a known shape, then the resolution function may be determined through a deconvolution procedure. It is common to use a step, or edge, to obtain a representation of the *cumulative resolution function* (10.3).

Note 2 to entry: If there is more than one simultaneous input measurand, for example in a lateral or volume *map* (8.57), or an energy and angle resolving spectrometer, then the feature is a point in the multi-dimensional input measurand space.

Note 3 to entry: The resolution function may change with the absolute value of the input measurand or measurands.

Note 4 to entry: The signal may be processed, smoothed or fitted to correct for background signal, non-linearity and to reduce *noise* (3.19) before the resolution function is extracted.

Note 5 to entry: In mass spectrometry, the peak shape of a single *ion species* (3.36) provides the mass resolution function directly.

10.3
cumulative resolution function

normalised integral of a one-dimensional *resolution function* (10.2) over the input *measurand* (3.3) value

Note 1 to entry: It is common to use a step, or edge, to obtain an experimental representation of the cumulative resolution function. The signal may be processed, smoothed or fitted to correct for background signal, non-linearity and reduce *noise* (3.19) before the cumulative resolution function is extracted.

10.4
relative resolution

ratio of *resolution* (10.1) at a specified *measurand* (3.3) value to that measurand value

10.5
resolving power

ratio of a specified *measurand* (3.3) value to the *resolution* (10.1) at that measurand value

10.6
resolution of a spectrometer
spectrometer resolution

<angle, energy, frequency, mass, time, velocity, wavelength, wavenumber> contribution of the spectrometer to the measured *resolution* (10.1)

Note 1 to entry: See *relative resolution of a spectrometer* (10.7) and *resolving power of a spectrometer* (10.8).

Note 2 to entry: It can be convenient to specify the *energy resolution* (10.24) of an *electron spectrometer* (12.58), the *mass resolution* (10.25) of a mass spectrometer, or the wavelength resolution of an optical spectrometer.

Note 3 to entry: In practice, the spectrometer resolution can be deduced using a source with an emission line of known width, usually chosen to be as narrow as possible.

Note 4 to entry: Designs of spectrometer generally maintain the resolution either to be constant throughout the spectrum or to be proportional to the energy, mass, or wavelength being scanned. For the former, the *resolution* (10.1) is a useful term whereas, for the latter, the *relative resolution* (10.4) and *resolving power* (10.5) are more useful.

10.7
relative resolution of a spectrometer

<angle, energy, frequency, mass, time, velocity, wavelength, wavenumber> ratio of the *resolution of a spectrometer* (10.6) at a specified *measurand* (3.3) value to that measurand value

Note 1 to entry: See *resolving power of a spectrometer* (10.8).

Note 2 to entry: The *relative resolution* (10.4) of a spectrometer is the reciprocal of the resolving power of a spectrometer.

Note 3 to entry: It can be convenient to specify the relative *energy resolution* (10.24) of an *electron spectrometer* (12.58), the relative *mass resolution* (10.25) of a mass spectrometer, or the relative wavelength resolution of an optical spectrometer.

Note 4 to entry: In practice, the relative resolution of a spectrometer can be deduced using a source with an emission line of known width, usually chosen to be as narrow as possible.

Note 5 to entry: Designs of spectrometer generally maintain the resolution either to be constant throughout the spectrum or to be proportional to the energy, mass, or wavelength being scanned. For the former, the term resolution is useful whereas, for the latter, the relative resolution or *resolving power* (10.5) is more useful.

Note 6 to entry: The relative resolution is often expressed as a percentage.

10.8
resolving power of a spectrometer

<angle, energy, frequency, mass, time, velocity, wavelength, wavenumber> ratio of a specified *measurand* (3.3) value to the *resolution of a spectrometer* (10.6) at that measurand value

Note 1 to entry: See *relative resolution of a spectrometer* (10.7).

Note 2 to entry: The *resolving power* (10.5) of a spectrometer is the reciprocal of the relative resolution of a spectrometer.

Note 3 to entry: It can be convenient to specify the energy-resolving power of an *electron spectrometer* (12.58), the mass-resolving power of a mass spectrometer, or the wavelength-resolving power of an optical spectrometer.

Note 4 to entry: In practice, the spectrometer resolving power can be deduced using a source with an emission line of known width, usually chosen to be as narrow as possible.

Note 5 to entry: Designs of spectrometer generally maintain the *resolution* (10.1) either to be constant throughout the spectrum or to be proportional to the energy, mass, or wavelength being scanned. For the former, the resolution is a useful term whereas, for the latter, the *relative resolution* (10.4) and resolving power are more useful.

10.9
FWHM resolution

resolution (10.1) expressed as the full width of a *resolution function* (10.2) at 50 % of its maximum value

Note 1 to entry: This is a commonly-used resolution criterion. It is approximately 2.355 times the standard deviation of a Gaussian resolution function.

10.10
X % peak width resolution

resolution (10.1) expressed as the full width of a *resolution function* (10.2) at *X* % of its maximum value

Note 1 to entry: This resolution criterion is used in mass spectrometry. The value of *X* shall be specified, *X* = 10 is the most frequently used value.

Note 2 to entry: see *peak width* (3.28).

10.11
12/88 resolution

resolution (10.1) expressed as the distance between the 12 % and 88 % intensity points in a *cumulative resolution function* (10.3) obtained across a well-defined edge or step

Note 1 to entry: This resolution criterion is frequently used for *depth resolution* (10.18) and *energy resolution* (10.24). It is equivalent to the FWHM, or approximately 2,355 times, the standard deviation of a Gaussian *resolution function* (10.2).

10.12
16/84 resolution

resolution (10.1) expressed as the distance between the 16 % and 84 % intensity points in a *cumulative resolution function* (10.3) obtained across a well-defined edge or step

Note 1 to entry: This resolution criterion is frequently used for *depth resolution* (10.18) and *lateral resolution* (10.17). It is equivalent to twice the standard deviation of a Gaussian *resolution function* (10.2).

10.13
20/80 resolution

resolution (10.1) expressed as the distance between the 20 % and 80 % intensity points in a *cumulative resolution function* (10.3) obtained across a well-defined edge or step

Note 1 to entry: This resolution criterion is frequently used for *lateral resolution* (10.17). It is equivalent to approximately 1.68 times the standard deviation of a Gaussian *resolution function* (10.2).

10.14
spatial resolution

length which describes the minimum distinguishable distance between features or areas in a chemical or topographic *map* (8.57) or *line scan* (8.56) in a specified direction

Note 1 to entry: *Depth resolution* (10.18) and *lateral resolution* (10.17) are specific types of spatial resolution

10.15
useful spatial resolution

<SIMS> *spatial resolution* (10.14) obtained in practice

Note 1 to entry: The spatial resolution of a *map* (8.57) is poorer than the primary-ion *beam diameter* (8.30) as a result of either the requirement to maintain the damage level below a limit set by the integrity of the data or the requirement to record sufficient signal when the sample is being consumed during analysis.

10.16
observed interface width

<AES, XPS, SIMS> distance over which a 16 % to 84 %, or 84 % to 16 %, change in *signal intensity* (3.17) is measured at the junction of two dissimilar matrices, the thicknesses of which are more than six times that distance

Note 1 to entry: The change in signal intensity should be quoted with the observed interface width.

Note 2 to entry: The observed interface width includes contributions from the sample such as interfacial roughness, mixing or diffusion as well as contributions from instrument resolution.

10.17
lateral resolution

length which describes the minimum distinguishable distance between features or areas in a chemical or topographic *map* (8.57) or *line scan* (8.56) in the plane of the sample *surface* (3.2)

Note 1 to entry: See also *resolution* (10.1), *point spread function* (10.21), *line spread function* (10.23), *edge spread function* (10.22) and *spatial resolution* (10.14).

Note 2 to entry: In practice, lateral resolution can be realized as the *FWHM resolution* (10.9) of the intensity distribution for a region which has lateral dimensions less than a quarter of the lateral resolution, or the distance between the *12/88 resolution* (10.11) in a *lateral profile* (3.31) across a well-defined material edge. These two values are equivalent for a Gaussian *resolution function* (10.2). For other resolution functions, other criteria may be more appropriate. For a step function, the distance between the *20/80 resolution* (10.13) or the *16/84 resolution* (10.12) in a lateral profile is also used.

Note 3 to entry: The direction in the lateral plane should be stated. For a radially symmetric beam with *incidence angle* (8.1) X°, lateral resolution in the azimuthal direction of the beam is a factor sec(X) larger than the orthogonal lateral resolution.

Note 4 to entry: Lateral resolution should not be confused with the *step size* (3.13), pixel pitch or pixel density of a *map* (8.57).

10.18
depth resolution

quantity which describes the minimum distinguishable depth between chemical features or regions in a direction normal to the sample surface

Note 1 to entry: See also *resolution* (10.1) and *spatial resolution* (10.14).

Note 2 to entry: In practice, the depth resolution can be realized as the *FWHM resolution* (10.9), in depth, of the intensity distribution for a *delta layer* (5.12) or the *16/84 resolution* (10.12) in a *depth profile* (3.32) across a well-defined sharp *interface* (3.1). Other measures may be used depending upon requirements.

10.19
instrumental depth resolution

contribution to *depth resolution* (10.18) arising from parameters of the instrument

Note 1 to entry: In *MEIS* (17.3) and *RBS* (17.4) this arises from the *energy resolution* (10.24) of the spectrometer.

Note 2 to entry: In *sputter depth profiling* (9.1), these parameters involve the system alignment and can include the *ion species* (3.36), energy, and *angle of incidence* (8.1) as well as the option to rotate the sample while *sputtering* (9.3).

10.20
depth resolution parameter

parameter which can be used as a coefficient in an analytic fit to a measured *compositional depth profile* (3.33) or a qualitative way of describing that profile

EXAMPLE Standard deviation for a Gaussian *resolution function* (10.2), full width at half maximum intensity for any bell-shaped resolution function and *decay length* (4.31) for an exponentially increasing or decreasing region of the resolution function.

Note 1 to entry: See *depth resolution* (10.18).

Note 2 to entry: Standard deviations can be used for any bell-shaped curve. If parameters are measured for a step change in composition, care shall be taken that the depth range for the measurements is large enough to ensure that the signal becomes constant with depth on either side of the step.

Note 3 to entry: Parameter definitions should be used consistently.

10.21
point spread function
PSF
normalised distribution of *signal intensity* (3.17) in a *chemical mapping* (8.58) system resulting from a well-defined point feature

Note 1 to entry: For direct measurement of a PSF the feature should be much smaller than the width of the PSF. If the feature is larger than the width of the PSF, but has a known shape, then the *resolution function* (10.2) may be determined through a deconvolution procedure. The signal may be processed, smoothed or fitted to correct for background signal, non-linearity and reduce *noise* (3.19) before the resolution function is extracted.

Note 2 to entry: Identical to the two-dimensional or three-dimensional spatial resolution function.

10.22
edge spread function
ESF
normalised distribution of *signal intensity* (3.17) in a *chemical mapping* (8.58) system resulting from a well-defined edge in a direction orthogonal to that edge

Note 1 to entry: To obtain an experimental representation of the ESF, it is usual to acquire several traces in order to select a trace that exhibits no structure or peaks within the range used. The signal may be processed, smoothed or fitted to correct for background signal, non-linearity and reduce *noise* (3.19) before the ESF is extracted.

Note 2 to entry: See also *point spread function* (10.21), *line spread function* (10.23) and *cumulative resolution function* (10.3).

10.23
line spread function
LSF
normalised distribution of *signal intensity* (3.17) in a *chemical mapping* (8.58) system resulting from a well-defined thin line in a direction orthogonal to that line

Note 1 to entry: To obtain an experimental representation of the LSF, it is usual to acquire several traces in order to select a trace that exhibits no structure or peaks within the range used. The signal may be processed, smoothed or fitted to correct for background signal, non-linearity and reduce *noise* (3.19) before the LSF is extracted.

Note 2 to entry: See also *point spread function* (10.21).

10.24
energy resolution
quantity which describes the minimum distinguishable energy separation between peaks or regions in an energy spectrum

Note 1 to entry: In practice, energy *resolution* (10.1) can be realized as the *FWHM resolution* (10.9) of a monochromatic particle beam or the distance between the *12/88 resolution* (10.11) in a scan across a part of the spectrum containing a well-defined step function, such as the Ag Fermi edge in XPS. These two values are equivalent for a Gaussian *resolution function* (10.2). For other instruments and systems, other criteria may be more appropriate.

10.25
mass resolution
quantity which describes the minimum distinguishable *m/z* (20.1) separation between peaks in a *mass spectrum* (20.58) or the minimum distinguishable mass separation between signals in an *ion scattering spectrum* (18.23)

Note 1 to entry: In practice, mass *resolution* (10.1) in a mass spectrum can be realized as the *FWHM resolution* (10.9) of a peak from a single *ion species* (3.36). The *10 % peak width resolution* (10.10) or other criteria are also used. The criterion used should be stated.

Note 2 to entry: The IUPAC definition of mass resolution[11] in a mass spectrum is equivalent to the ISO and IUPAC definitions of mass *resolving power* (10.5). ISO TC201 maintains the distinction between resolution and resolving power for mass spectrometry in surface analysis to avoid confusion in surface analytical terminology.

11 Terms related to electron spectroscopy methods

11.1
Auger electron spectroscopy
AES
method in which an *electron spectrometer* (12.58) is used to measure the energy distribution of *Auger electrons* (12.32) emitted from a *surface* (3.2)

Note 1 to entry: An electron beam in the energy range 2 keV to 30 keV is often used for excitation of the Auger electrons. Auger electrons can also be excited with X-rays, ions, and other sources but the term Auger electron spectroscopy, without additional qualifiers, is usually reserved for electron-beam-induced excitation. Where an X-ray source is used, the Auger electron energies are referenced to the *Fermi level* (12.9) but, where an electron beam is used, the reference can either be the Fermi level or the *vacuum level* (12.10). Spectra, conventionally, can be presented in the *direct* (12.68) or *differential* (12.69) forms.

11.2
angle-resolved AES
ARAES
angle-dependent AES
method in which *Auger electron* (12.32) intensities are measured as a function of the *angle of emission* (8.5)

11.3
reflection electron energy loss spectroscopy
REELS
method in which an *electron spectrometer* (12.58) is used to measure the energy distribution of electrons quasi-elastically scattered by atoms at or in a surface layer and the associated *electron energy loss spectrum* (12.71)

Note 1 to entry: See *elastic peak electron spectroscopy* (11.4).

11.4
elastic peak electron spectroscopy
EPES
method in which an *electron spectrometer* (12.58) is used to measure the energy, intensity, and/or energy broadening distribution of quasi-elastically scattered electrons from a solid or liquid *surface* (3.2)

Note 1 to entry: See *recoil effect* (12.44) and *reflection electron energy loss spectroscopy (REELS)* (11.3).

Note 2 to entry: An electron beam in the energy range 100 eV to 3 keV is often used for this kind of spectroscopy.

Note 3 to entry: In general, electron sources with energy spreads that are less than 1 eV are required to provide adequate information.

Note 4 to entry: EPES is often an auxiliary method of *AES* (11.1) and REELS, providing information on the composition of the surface layer. EPES is suitable for the experimental determination of the *inelastic mean free path* (12.41), the electron *differential elastic scattering cross section* (4.9), and the *surface excitation parameter* (12.43).

11.5
angle-resolved EPES
AREPES
<EPES> method involving *EPES* (11.4) measurements as a function of the *scattering angle* (8.4)

11.6
X-ray photoelectron spectroscopy
XPS

method in which an *electron spectrometer* (12.58) is used to measure the energy distribution of photoelectrons and *Auger electrons* (12.32) emitted from a *surface* (3.2) irradiated by X-ray photons

Note 1 to entry: X-ray sources in common use are unmonochromated Al Kα and Mg Kα X-rays at 1 486,6 eV, and 1 253,6 eV, respectively. Modern instruments also use monochromated Al Kα X-rays. Some instruments make use of various X-ray sources with other anodes or of *synchrotron radiation* (7.1).

Note 2 to entry: *EP-XPS* (11.11), *NAP-XPS* (11.12) and *HAXPES* (11.10) are variants of XPS.

11.7
angle-resolved XPS
ARXPS
angle-dependent XPS

procedure in which X-ray photoelectron intensities are measured as a function of the *angle of emission* (8.5)

Note 1 to entry: This procedure is often used to obtain information on the distribution with depth of different elements or compounds in a layer approximately 5 nm thick at the *surface* (3.2).

11.8
ultraviolet photoelectron spectroscopy
UPS

method in which an *electron spectrometer* (12.58) is used to measure the energy distribution of photoelectrons emitted from a *surface* (3.2) irradiated by ultraviolet photons

Note 1 to entry: Ultraviolet sources in common use include various types of discharges that can generate the resonance lines of various gases (e.g. the He I and He II emission lines at energies of 21,2 eV and 40,8 eV, respectively). For variable energies, *synchrotron radiation* (7.1) is used.

Note 2 to entry: Angle-resolved UPS is termed *ARPES* (11.9).

11.9
angle-resolved photoelectron spectroscopy
ARPES

procedure in which photoelectron intensities are measured as a function of both the *angle of emission* (8.5) and the azimuthal angle

Note 1 to entry: This procedure is often used to obtain information on the electronic and structural properties of a single crystal *surface* (3.2) using either VUV or X-ray irradiation.

11.10
hard X-ray photoemission spectroscopy
hard X-ray photoelectron spectroscopy
HAXPES

method in which an *electron spectrometer* (12.58) is used to measure the energy distribution of photoelectrons and *Auger electrons* (12.32) emitted from a *surface* (3.2) irradiated by X-ray photons with energies greater than 2 140 eV

Note 1 to entry: See also *X-ray photoelectron spectroscopy* (11.6).

Note 2 to entry: The lower limit of photon energies for HAXPES is defined as the lowest energy achievable with a Si(111) double crystal monochromator in accordance with Reference [12].

11.11
extended pressure X-ray photoelectron spectroscopy
EP-XPS

method in which an *electron spectrometer* (12.58) is used to measure the energy distribution of photoelectrons and *Auger electrons* (12.32) emitted from a solid or liquid *surface* (3.2) irradiated by X-ray photons in the presence of gas with a pressure greater than 0,001 mbar and smaller than 1 mbar.

Note 1 to entry: See also *X-ray photoelectron spectroscopy* (11.6) and *near ambient pressure X-ray photoelectron spectroscopy* (11.12).

Note 2 to entry: 1 mbar = 10^{-4} MPa = 100 Pa; 1 MPa = 1 N/mm^2.

11.12
near ambient pressure X-ray photoelectron spectroscopy
NAP-XPS

method in which an *electron spectrometer* (12.58) is used to measure the energy distribution of photoelectrons and *Auger electrons* (12.32) emitted from a solid or liquid *surface* (3.2) or a gas irradiated by X-ray photons in the presence of gas with a pressure greater than 1 mbar and smaller than 1 000 mbar

Note 1 to entry: See also *X-ray photoelectron spectroscopy* (11.6) and *extended pressure X-ray photoelectron spectroscopy* (11.11).

Note 2 to entry: 1 mbar = 10^{-4} MPa = 100 Pa; 1 MPa = 1 N/mm^2.

11.13
Auger photoelectron coincidence spectroscopy
APECS

detection of an *Auger electron* (12.32) and a core-level photoelectron, emitted from a solid irradiated by mono-energetic X-rays, within a sufficiently short time that the Auger electron arises from the decay of the particular core-*hole* (3.61) associated with the photoelectron

11.14
photoelectron emission microscopy
PEEM

method in which the spatial or angular distributions of electrons emitted from a surface through the *photoelectric effect* (12.7) are simultaneously measured

Note 1 to entry: Photoelectron emission microscopy is a form of electron microscopy in which emitted photoelectrons are magnified and refocussed onto a position sensitive detector.

Note 2 to entry: The sample is typically held at a high negative potential and UV irradiation employed to reduce the spread in photoelectron energies and reduce *chromatic aberrations* (7.23).

Note 3 to entry: PEEM instruments can include electron energy filters which enable direct imaging of the spatial or angular distributions of specific photoelectron energies.

Note 4 to entry: PEEM may be used to measure the spatial distributions of *work function* (12.12), surface chemistry, electronic structure and magnetic properties with *spatial resolution* (10.14) significantly better than 100 nm.

Note 5 to entry: The acronym X-PEEM indicates that X-rays are used as the photoelectron excitation source.

11.15

X-ray standing waves

XSW

method based on the interference of X-rays that occurs near the Bragg condition at the surface of a crystalline solid which leads to intensity variations in yields of photoelectrons as the Bragg condition is scanned by tilting the sample or changing the X-ray energy

Note 1 to entry: Intensity nodes are scanned from one lattice plane to the next as the Bragg condition is altered. Atomic positions in the crystalline lattice can be determined from comparisons of measured scans of photoelectron intensity with calculated scans from dynamical scattering theory.

12 Terms related to electron spectroscopy analysis

12.1

primary electron

electron extracted from a source and directed at a sample

Note 1 to entry: See *secondary electron* (12.2).

12.2

secondary electron

electron, generally of low energy, leaving a *surface* (3.2) as a result of an excitation induced by an incident electron, photon, ion, or neutral particle

Note 1 to entry: By convention, electrons with energies ≤ 50 eV are considered as secondary electrons unless otherwise specified. Calculations of the energy distribution of the electrons emitted from a surface show that 50 eV is a useful cut-off energy to contain most of the electrons. The cut-off is artificial, and secondary electrons with energies greater than 50 eV usually exist. This convention is not usually observed for *GDS* (15.1).

12.3

backscattered electron

<AES, EELS> electron, originating in the incident beam, which is emitted after interaction with the sample

Note 1 to entry: By convention, an electron with energy greater than 50 eV can be considered as a backscattered electron.

Note 2 to entry: By convention, the incident beam is often called the *primary beam* (8.10) and the backscattered electrons are often referred to as the backscattered *primary electrons* (12.1).

12.4

backscattering yield

backscattering coefficient

η

<AES> ratio of the total number of electrons emitted from the sample with energies greater than 50 eV to the total number of electrons incident at a given energy and *angle of incidence* (8.1)

Note 1 to entry: See *secondary-electron yield* (12.5), *total secondary-electron yield* (12.6), and *backscattering correction factor* (12.53).

12.5

secondary-electron yield

secondary-electron emission coefficient

δ

<AES> ratio of the total number of electrons emitted from a sample with energies less than 50 eV to the total number of electrons incident at a given energy and *angle of incidence* (8.1)

12.6
total secondary-electron yield

σ

<AES> ratio of the total number of electrons emitted from a sample to the total number of electrons incident at a given energy and *angle of incidence* (8.1):

$$\sigma = \delta + \eta$$

where δ is the *secondary-electron yield* (12.5) and η is the backscattering coefficient

Note 1 to entry: See *backscattering yield* (12.4) and secondary-electron yield.

Note 2 to entry: The total secondary-electron yield is often simply called the secondary-electron yield. This leads to confusion with the term of that name which is restricted to *secondary electrons* (12.2), with energies ≤50 eV.

12.7
photoelectric effect

interaction of a photon with bound electrons in atoms, molecules and solids, resulting in the production of one or more photoelectrons

12.8
photoemission

emission of electrons from atoms or molecules caused by the *photoelectric effect* (12.7)

12.9
Fermi level

thermodynamic work required to add one electron to a material

Note 1 to entry: See *vacuum level* (12.10).

Note 2 to entry: For insulators and semiconductors, the Fermi level is usually between the valence and conduction bands.

12.10
vacuum level

electric potential of the vacuum at a point in space

Note 1 to entry: See *Fermi level* (12.9).

Note 2 to entry: In electron spectroscopy, the point in space is taken at a sufficiently large distance outside the sample such that electric fields caused by different *work functions* (12.12) of different parts of the *surface* (3.2) are zero or extremely small.

12.11
standard vacuum level

electric potential 4,500 eV above the *Fermi level* (12.9)

Note 1 to entry: See *vacuum level* (12.10).

Note 2 to entry: The Fermi level is an absolute level to which electron *kinetic energies* (3.35) can be accurately referenced. Historically, in *AES* (11.1), the electron energies have not been referenced to the Fermi level but, instead, have been referenced to the instrument vacuum level. This level varies from instrument to instrument and does not provide a consistent reference level. However, most reported *Auger electron* (12.32) kinetic energies have been referenced to the vacuum level, and most analysts are familiar with the variations that occur from one instrument to another for energies referenced in this way. By convention, the standard vacuum level is defined, as above, to be a consistent reference level close to the value for typical instrument vacuum levels. Energies referenced to the standard vacuum level are consistent and are within approximately 1 eV of those referenced to individual instrument vacuum levels.

12.12
work function

potential difference for electrons between the *Fermi level* (12.9) and the maximum potential just outside a specified *surface* (3.2)

Note 1 to entry: The work functions of the different crystal facets of a single crystal in general differs from one another. These work functions also change with the state of cleanness of the crystal surfaces.

Note 2 to entry: A polycrystalline surface exhibits an average work function which depends on the types of exposed constituent single-crystal facets and their areas.

12.13
photoelectric work function

minimum photon energy required to liberate an electron from the surface of a conducting solid by absorption of that photon

Note 1 to entry: The *work functions* (12.12) of the different facets of the crystals in a polycrystalline solid in general differ from one another. There are localized or patch electric fields close to the surfaces of these facets even if the region distant from the solid is, on the average, field-free. Patch fields in the vicinity of the facet with the lowest work function retards photo-emitted electrons. These electrons can only be detected if a suitable extraction field is applied. Without an extraction field, the measured photoelectric work function becomes equivalent to the area-averaged work function.

Note 2 to entry: If the surface is immersed in an extraction field, the minimum photon energy, and hence the measured photoelectric work function are both reduced. The extent of the reduction depends on the extraction field strength and the size of the different facets.

Note 3 to entry: Work functions are often measured in *photoemission* (12.8) experiments where the work function is taken as equal to the photon energy minus the difference between the lowest energy electrons emitted and those emitted characteristic of the *Fermi level* (12.9). For such experiments, photons from the He I ultraviolet emission line are commonly used. The lowest energy measured depends on the presence of an extraction field. In many publications there is confusion between the measured lowest energy in the spectrum and lowest energy after deconvolving the *spectrometer resolution* (10.6). Ignoring the finite *energy resolution* (10.24) leads to an erroneously low value of the work function.

12.14
thermionic work function

parameter describing the apparent *work function* (12.12) of a solid that controls the electronic current density, J, emitted from a conductor at temperature T, and equal to $-kT \ln(J/AT^2)$, where k is Boltzmann's constant and A is Richardson's constant

Note 1 to entry: For polycrystalline solids, the thermionic work function is close to the minimum work function of the crystallites present.

Note 2 to entry: Richardson's constant, A, is given by $A = (4\pi mk^2e)/h^3 = 1{,}201\ 73 \times 10^6\ \mathrm{Am}^{-2}\mathrm{K}^{-2}$, where m and $-e$ are the mass and charge on the electron, respectively, and h is Planck's constant.

12.15
Einstein's photoelectric equation

formula in which the *kinetic energy* (3.35) of an electron, emitted from a conductor illuminated by monochromatic photons, is given by the photon energy minus the *work function* (12.12) of the surface from which the photoelectron is emitted

12.16
binding energy

energy expended in removing an electron from a given electronic level to the *Fermi level* (12.9) of a solid or to the *vacuum level* (12.10) of a free atom or molecule

Note 1 to entry: See also *binding energy scale* (12.73)

12.17

chemical effects

<AES, EELS, XPS> changes in the shape of a measured spectrum, or in the *peak energy* (12.72) for an element, arising from chemical bonding

12.18

chemical shift

<AES, EELS, XPS> change in *peak energy* (12.72) arising from a change in the chemical environment of the atom

12.19

multiplet splitting

<AES> splitting of an *Auger electron* (12.32) line into two or more components, caused by the interactions of the atomic vacancies created by the *Auger process* (12.30)

12.20

multiplet splitting

exchange splitting

<XPS> splitting of a photoelectron line caused by the interaction of the unpaired electron, created by *photoemission* (12.8), with other unpaired electrons in the atom

12.21

intrinsic lineshape

natural lineshape

<AES, UPS, XPS> *lineshape* (3.27) of a spectral feature after removal of all instrumental contributions

Note 1 to entry: A background can or cannot be removed from the lineshape of interest, depending on the circumstances. The procedure for determination of the intrinsic lineshape may be complex and should therefore be clearly stated.

Note 2 to entry: In *AES* (11.1), a background due to *inelastic scattering* (4.2), *secondary electrons* (12.2), or *backscattered electrons* (12.3) may be removed. See *inelastic background* (12.46) and *Sickafus background* (12.87).

Note 3 to entry: In *XPS* (11.6), a background due to other *photoemission* (12.8) processes and to inelastic scattering processes in the sample may be removed. See inelastic background.

12.22

intrinsic linewidth

natural linewidth

<AES, UPS, XPS> full width at half maximum intensity of a spectral feature for a particular transition after removal of the background and all instrumental terms including the contribution of the exciting source

Note 1 to entry: The measured linewidth is determined from the measured *lineshape* (3.27) which is a convolution of the *intrinsic lineshape* (12.21) with broadening contributions of the sample and of the instrument *resolution function* (10.2) [e.g. the linewidth of the X-ray source in *XPS* (11.6) and spectrometer *energy resolution* (10.24) in both *AES* (11.1) and XPS].

12.23

chemical state

<AES, EELS, UPS, XPS> state of an atom arising from its chemical interaction with neighbouring atoms in a molecule, compound, solid, liquid, or gas that leads to a characteristic energy or feature observable in electron spectroscopy

Note 1 to entry: Examples of features observed are satellite peaks, shifts in the *peak energy* (12.72) positions, changes in the *lineshape* (3.27), and changes in the *characteristic electron energy losses* (12.40) spectra at lower *kinetic energies* (3.35) than the photoelectron or *Auger electron* (12.32) peaks.

Note 2 to entry: A full description of chemical state is denoted by the complete set of electronic states and the electron configuration in the core of the atom providing the signal, as well as the electronic and physical structure (including charge distribution, density of electronic states, and electronic configuration) local to this atom.

Note 3 to entry: The chemical state of a selected atom is determined by its interaction (e.g. chemical-bonding iconicity or covalency) with nearby atoms, most importantly its nearest neighbours. It is determined by the oxidation number of an atom in a compound, by the coordination (mostly by its stereo structure and coordination number) and by the differences in the kinds of element in the position of the first-nearest neighbour, second-nearest neighbour, and so on. These all affect the effective charge and spin state of the selected atom.

Note 4 to entry: Different or distinguishable sets of chemical properties (different chemical states) of a *chemical species* (3.5) can occur as a consequence of differing valence-band electronic structures, including charge distributions and electronic configurations, localized on the given chemical species. In *XPS* (11.6), the term chemical state is mostly used for characterizing measured binding energies, Auger electron kinetic energies, and *Auger parameters* (12.80) with different oxidation states of a given element in different chemical compounds, e.g. the Cr III oxidation state in Cr_2O_3 and $Cr(OH)_3$. In *AES* (11.1), the term chemical state is often used to characterize the shape of the *Auger electron spectrum* (12.70) for the atoms of an element in different chemical environments, e.g. the shape of the carbon Auger electron spectrum for graphite and for various carbides. Differences in the chemical properties of a chemical species in various environments can result in differences in the respective peak energies, satellite structures, *lineshapes* (3.27), or *energy loss* (4.3) features in the corresponding Auger or photoelectron spectra.

Note 5 to entry: The quantum theory of atoms in molecules defines an atom in a molecule or crystal as a bounded region of real space, an open quantum system. However, there is no wave function for the atom; they are only for the total system. Hence, there is no state designation for the atom, only for the total system. What physics provides are expectation values of all the observables, measurable or otherwise, for the bound atom. In this sense, its state is defined within the total system by the net charge and energy of the atom and how changes of charge and energy are reflected in the observed (e.g. Auger or photoelectron) spectra.

12.24
surface core-level shift

energy shift observed in core-level photoelectron spectroscopy arising from the reduced coordination of the *surface* (3.2) or near-surface atoms compared to bulk atoms

Note 1 to entry: Surface core level shifts are often observed for single crystals and nanoparticles and depend on the crystal surface exposed. Shifts can be to lower or higher binding energy depending on the band structure of the bulk solid. For the outermost atom layer, the shift can be as high as 0,4 eV. In XPS, the sampling depth is generally many atom layers when photoelectrons are detected with *emission angles* (8.5) at, or close to, the surface normal. The shift for the outermost atom layer is thus seen most clearly at near-grazing emission angles. Separate energy shifts can be detected for the second and third atom layers from the surface.

12.25
interface core-level shift

energy shift observed in core-level photoelectron spectroscopy arising from the changed bonding and/or from the displacements of atoms from their bulk positions near an *interface* (3.1) between two materials

Note 1 to entry: See *surface core-level shift* (12.24).

12.26
photoionization cross section

total *ionization cross section* (4.26) for an incident photon of a given energy interacting with a material to produce one or more photoelectrons from all sub-shells that are energetically accessible

Note 1 to entry: See *ionization cross section* (4.26) and *sub-shell photoionization cross section* (12.27).

12.27
sub-shell photoionization cross section

cross section (4.7) for an incident photon interacting with a material to produce one or more photoelectrons from a given sub-shell

Note 1 to entry: See *photoionization cross section* (12.26).

Note 2 to entry: Photoionization from one sub-shell can lead to *shakeup* (12.51) or *shakeoff* (12.52) of electrons from other shells.

12.28
asymmetry parameter
β
<XPS> factor which characterizes the intensity distribution, $L(\gamma)$, of photoelectrons ejected by unpolarized X-rays from isolated atoms in a direction γ from the incident X-ray direction in accordance with

$$L(\gamma)=1+\frac{1}{2}\beta\left[\frac{3}{2}\left(\sin^2\gamma\right)-1\right]$$

Note 1 to entry: This formula relates to gases and is modified by the effects of *elastic scattering* (4.1) when applied to solids. At the *magic angle* (12.29), $L(\gamma)$ = 1.

12.29
magic angle
<XPS> angle at which the spectrometer entrance axis is aligned at 54,7° to the direction of the X-rays at the sample *surface* (3.2)

Note 1 to entry: At the magic angle, using the simple dipole theory for the angular distribution of the photoelectrons emitted from an atom irradiated by unpolarized X-rays, it is predicted that the intensity per unit solid angle is the same as the intensity that would be obtained if the scattering were isotropic.

12.30
Auger process
relaxation (3.57), by electron emission, of an atom with a vacancy in an inner electron shell

Note 1 to entry: See *Auger de-excitation* (3.72), *Auger electron* (12.32), and *Auger transition* (12.33).

Note 2 to entry: The emitted electrons have characteristic energies, defined by the Auger transition.

12.31
Auger electron yield
probability that an atom with a vacancy in a particular inner shell relaxes by an *Auger process* (12.30)

12.32
Auger electron
electron emitted from atoms in the *Auger process* (12.30)

Note 1 to entry: See *Auger transition* (12.33).

Note 2 to entry: Auger electrons can lose energy by *inelastic scattering* (4.2) as they pass through matter. Measured Auger electron spectra are therefore generally composed of a peak structure of unscattered Auger electrons superimposed on a background of inelastically scattered Auger electrons with intensities extending to lower kinetic energies, and on backgrounds arising from other processes.

Note 3 to entry: Auger electrons can change their direction of propagation by *elastic scattering* (4.1) as they pass through matter.

12.33
Auger transition
Auger process (12.30) involving designated electron shells or sub-shells

Note 1 to entry: The three shells involved in the Auger process are designated by three letters. The first letter designates the shell containing the initial vacancy and the last two letters designate the shells containing electron vacancies left by the Auger process (e.g. KLL or LMN). When a valence electron is involved, the letter V is used (e.g. LMV or KVV). When a particular sub-shell involved is known, this can also be indicated (e.g. KL_1L_2). Coupling terms can also be added, where known, to indicate the final atomic state (e.g. $L_3M_{4,5}M_{4,5};{}^1D$).

Note 2 to entry: More complicated Auger processes (such as multiple initial ionizations and additional electronic excitations) can be designated by separating the initial and *final states* (3.56) by a hyphen (e.g. LL-VV, or K-VVV).

Note 3 to entry: When an Auger process involves an electron from the same principal shell as the initial vacancy (e.g. L_1L_2M), it is referred to as a *Coster-Kronig transition* (12.36). If all electrons are from the same principal shell (e.g. $M_1M_2M_3$) the process is called a *super Coster-Kronig transition* (12.37).

12.34
Auger transition rate
quotient of the probability for an *Auger process* (12.30) by time

12.35
interatomic Auger process
Auger transition (12.33) in which at least one of the final electron vacancies is localized in valence levels or molecular orbitals of atoms adjacent to the atom in which the initial vacancy occurred

12.36
Coster-Kronig transition
Auger process (12.30) involving an electron from the same principal shell as the initial vacancy

Note 1 to entry: See *Auger transition* (12.33) and *super Coster-Kronig transition* (12.37).

EXAMPLE $L_1L_2M_5$; $M_1M_2N_5$.

12.37
super Coster-Kronig transition
<AES, XPS> *Coster-Kronig transition* (12.36) in which the ejected electron is from the same principal shell as the initial vacancy

Note 1 to entry: See *Auger transition* (12.33).

EXAMPLE $M_2M_4M_5$; $N_5N_7N_7$.

12.38
Auger vacancy satellite
Auger transition (12.33) in which additional *spectator holes* (3.63) are present in the *initial state* (3.54) or the *final state* (3.56) for the transition

12.39
inelastic scattering cross section
<AES, EELS, XPS> *cross section* (4.7) for *inelastic scattering* (4.2) by an electron traversing a material

12.40
characteristic electron energy losses
inelastic scattering (4.2) of electrons in solids that produces a non-uniform *electron energy loss spectrum* (12.71) determined by the characteristics of the material

Note 1 to entry: See *plasmon* (12.47) and *surface plasmon* (12.48).

Note 2 to entry: The most probable characteristic losses arise from excitation of valence electrons. For some solids (e.g. non-transition metals), inelastic scattering is dominated by plasmon excitations. For other solids, the inelastic scattering can be due to a combination of plasmon excitation and single valence-electron excitations, and these excitations may not be distinguishable. Inelastic scattering can also occur through the excitation of core level electrons when this is energetically possible.

Note 3 to entry: The characteristic energy losses are most prominent in the energy loss range 0 eV to 100 eV.

Note 4 to entry: Characteristic electron energy loss peaks are often observed in association with other peaks in a spectrum [e.g. *Auger electron* (12.32) peaks, photoelectron peaks, and the peak arising from *elastic scattering* (4.1) of *primary electrons* (12.1)].

12.41
electron inelastic mean free path
average distance that an electron with a given energy travels between successive inelastic collisions

Note 1 to entry: See *attenuation length* (4.30).

12.42
elastic peak
quasi-elastic peak
peak in the electron spectrum, produced by quasi-elastically scattered electrons detected by an *electron spectrometer* (12.58)

Note 1 to entry: See *elastic peak electron spectroscopy, EPES* (11.4), *inelastic scattering* (4.2), *recoil effect* (12.44), and *reflection electron energy loss spectroscopy (REELS)* (11.3).

Note 2 to entry: All electrons that are scattered by atoms can be elastically scattered in the centre-of-mass frame, but *energy losses* (4.3) that are typically less than 1 eV can be observed in the laboratory frame. These losses are generally significantly less than the measured energy width of the electrons in a primary-electron beam. Historically, and more generally, the scattering has been called “elastic”; however, the term quasi-elastic is now often used if the small change in energy that occurs on scattering is important.

Note 3 to entry: The energy and the energy broadening of the quasi-elastic peak are influenced by the recoil of the scatterer atoms, the energy distribution of the primary (incident) electrons, the scattering geometry, the acceptance geometry, and the *response function* (7.13) of the electron spectrometer. The intensity of the elastic peak depends on the electron *differential elastic scattering cross section* (4.9) and on the total *cross section* (4.7) for inelastic electron scattering at the particular primary-electron *beam energy* (8.33) and in the given scattering geometry, including the probability of surface excitations.

12.43
surface excitation parameter
SEP
<AES, EPES, REELS, XPS> characteristic parameter in the exponential attenuation, describing the ratio of the intensity of a peak resulting from the presence of the *surface* (3.2), during a single crossing of a material surface, to that expected after traversing the same amount of material but in the absence of the surface

Note 1 to entry: If it is assumed that the SEP arises solely from surface excitations and that multiple surface excitations are governed by the Poisson stochastic process, the probability of experiencing n surface excitations is given by $(S^n/n!)[\exp(-S)]$, where S is the SEP. The SEP can then be interpreted as the average number of surface excitations during a single surface crossing, and the probability for not experiencing any surface excitation during that single surface crossing is given by $\exp(-S)$.

Note 2 to entry: The value of the SEP depends on the geometry of the experiment, and the contributions for incoming and for outgoing electrons in *EPES* (11.4) and *REELS* (11.3) can differ. The SEP decreases the intensities observed in REELS, EPES, *AES* (11.1), *XPS* (11.6), and similar types of spectroscopy.

Note 3 to entry: Surface excitation decreases the intensity of the *quasi-elastic peak* (12.42). It is important in REELS and EPES.

12.44
recoil effect
<EPES> effect resulting from the change in movement of a scatterer atom as a result of quasi-elastic electron scattering

Note 1 to entry: The energy shift and energy broadening of the *quasi-elastic peak* (12.42) for a scattered electron beam due to atomic recoil depend on the mass of the scatterer atom, the energy of the *primary electrons* (12.1), and the *scattering angle* (8.4). In addition, the energy broadening due to atomic recoil depends on the sample temperature. The quasi-elastic peak in *EPES* (11.4) for multicomponent materials contains contributions from each component. Recoil effects are most easily observable in electron spectra taken at a high *energy resolution* (10.24) with low atomic number scattering atoms. Hydrogen can be directly detected by its recoil shift.

12.45
effective attenuation length
<AES, XPS> parameter which, when introduced in place of the *inelastic mean free path* (12.41) into an expression derived for *AES* (11.1) and *XPS* (11.6) on the assumption that *elastic scattering* (4.1) effects are negligible for a given quantitative application, corrects that expression for elastic scattering effects

Note 1 to entry: See *attenuation length* (4.30).

Note 2 to entry: The effective attenuation length can have different values for different quantitative applications of AES and XPS. However, the most common use of effective attenuation length is in the determination of overlayer-film thicknesses from measurement of the changes of overlayer and substrate Auger-electron or photoelectron signal intensities after deposition of a film or as a function of the *emission angle* (8.5). For emission angles of up to about 60° (with respect to the surface normal), it is often satisfactory to use a single value of this parameter. For larger emission angles, the effective attenuation length can depend on this angle. Effective attenuation lengths have also been used in equations for determining the shell thicknesses of core-shell nanoparticles and for quantitative analysis (to describe the changes in AES and XPS signal intensities due to elastic scattering).

Note 3 to entry: Since there are different uses of this term, it is recommended that users specify clearly the particular application and the definition of the parameter for that application (e.g. by giving a formula or by providing a reference to a particular source). Effective attenuation lengths developed for one application should not be used for another application unless this usage has been validated.

12.46
inelastic background

intensity distribution in the spectrum for particles originally at one energy but which are emitted at lower energies due to one or more *inelastic scattering* (4.2) processes

Note 1 to entry: See *inelastic electron scattering background subtraction* (12.85), *Shirley background* (12.86), *Sickafus background* (12.87), and *Tougaard background* (12.88).

Note 2 to entry: For *AES* (11.1) and *XPS* (11.6), the inelastic background associated with a particular *Auger electron* (12.32) or photoelectron peak has been approximated by a measured *electron energy loss spectrum* (12.71) for which the incident-electron energy is close to the energy of the peak. The Tougaard background is also used. A simpler, but less accurate, inelastic background function is the Shirley background. Simple linear backgrounds have also been used, but these are much less accurate except for the XPS analysis of insulators.

12.47
plasmon
bulk plasmon
volume plasmon

excitation of valence-band electrons in a solid in which collective oscillations are generated

Note 1 to entry: See *characteristic electron energy losses* (12.40).

Note 2 to entry: Plasmon excitations are often observed as characteristic *energy loss* (4.3) peaks associated with other peaks in the spectrum such as those of any elastically scattered *primary electrons* (12.1), photoelectron peaks, *Auger electron* (12.32) peaks, and ionization edges.

Note 3 to entry: Plasmons are prominent in some materials and not others.

Note 4 to entry: Two types of plasmon are commonly observed: bulk plasmons associated with material remote from the *surface* (3.2) and *surface plasmons* (12.48) associated with material at the surface. When the term plasmon is used without a qualifier, the term refers to the bulk plasmon. Occasionally, *interface* (3.1) plasmons can be observed that are associated with interfaces. Bulk plasmon energies depend on the electronic structure of the material, and are roughly proportional to the square root of valence-band density. Surface plasmon energies are typically between 50 % and 90 % of bulk plasmon energies.

12.48
surface plasmon

excitation of conduction- or valence-band electrons in a solid or liquid, associated with the termination of the material at the *surface* (3.2), in which collective oscillations are generated

Note 1 to entry: See *characteristic electron energy losses* (12.40) and *plasmon* (12.47).

Note 2 to entry: Plasmon excitations are often observed as characteristic *energy loss* (4.3) peaks associated with other peaks or structures in the spectrum, such as those of any elastically scattered *primary electrons* (12.1), photoelectron peaks, *Auger electron* (12.32) peaks, and ionization edges. Surface plasmons are important for many optical measurements.

Note 3 to entry: Plasmons are prominent in some materials and not in others.

Note 4 to entry: Two types of plasmon are commonly observed: *bulk plasmon* (12.47) (often simply called plasmons), associated with material remote from a surface or *interface* (3.1), and surface plasmons, associated with a surface or interface. The bulk plasmon energy depends on the electronic structure of the material and is generally roughly proportional to the square root of the density of the valence-band electrons. The surface plasmon energy for a surface (i.e. a material-vacuum interface) is often approximately $(1/\sqrt{2})$ of the bulk plasmon energy for a planar surface; the actual ratio of the bulk and surface plasmon energies depends on the electronic structure of the material. For an interface between two materials, the surface plasmon energy depends on the electronic properties of each material. In the case of a thin oxide film on a free-electron-like metal, the surface plasmon energy of the metal is reduced compared to the value for the clean metal surface due to the presence of the oxide.

12.49
extrinsic plasmon

plasmon (12.47) excited as an electron travels through a condensed medium

Note 1 to entry: See *intrinsic plasmon* (12.50).

Note 2 to entry: The probability describing the number of extrinsic plasmons excited by the electron depends on the path length traversed and, for typical applications of *Auger electron spectroscopy* (11.1) and *X-ray photoelectron spectroscopy* (11.6) of a homogeneous sample, follows a Poissonian distribution for the parameter s/λ, where s is the path length and λ is the *inelastic mean free path* (12.41).

12.50
intrinsic plasmon

plasmon (12.47) excited at the same time as the excitation of a core-level photoelectron or an *Auger electron* (12.32) associated with the same locality as the excitation of the photoelectron or Auger electron

Note 1 to entry: See *extrinsic plasmon(12.49)*.

Note 2 to entry: The population of numbers of intrinsic plasmons observed follows a Poissonian distribution as a function of the number of multiple plasmons excited.

Note 3 to entry: Intrinsic plasmons are excited as a consequence of the suddenly created core *hole* (3.61). Usually, the core hole is assumed to have a stationary position and a finite lifetime. Interferences can take place between extrinsic and intrinsic excitations.

12.51
shakeup

<AES, XPS> multi-electron process in which an atom is left in an *excited state* (3.53) following a photoionization or *Auger electron* (12.32) process, so that the outgoing electron has a characteristic *kinetic energy* (3.35) slightly less than that of the parent photoelectron

Note 1 to entry: See *shakeoff* (12.52).

Note 2 to entry: Shakeup peaks are usually observed within 10 eV of the parent peak. However, for gases where the background is low, shakeup peaks have been identified at kinetic energies up to 100 eV less than that of the parent peak.

12.52
shakeoff

<AES, XPS> multi-electron process in which two or more electrons are emitted, partitioning between them the excess *kinetic energy* (3.35)

Note 1 to entry: See *shakeup* (12.51).

Note 2 to entry: Shakeup leads to peak structure at kinetic energies below that of a parent peak whereas shake off leads to a continuum background intensity, also at kinetic energies below that of the parent peak in the electron spectrum.

12.53
backscattering correction factor

<AES> factor equal to the ratio of the total Auger-electron current arising from ionizations in the sample caused by both the *primary electrons* (12.1) and the *backscattered electrons* (12.3) to the Auger-electron current arising directly from the primary electrons

Note 1 to entry: See *backscattering fraction* (12.54).

Note 2 to entry: The AES literature contains many references to “backscattering factor” but the use of this term is ambiguous. In some papers and books, the backscattering factor is the same as the backscattering correction factor, while in other papers and books the backscattering factor is identified as the backscattering fraction. In practice, this ambiguous usage generally does not cause misunderstanding since the backscattering correction factor (often denoted by R) is equal to unity plus the backscattering fraction (often denoted by r). To avoid misunderstanding, use of the term backscattering factor is deprecated.

Note 3 to entry: In simple theories, evaluations of the backscattering correction factor can be based on the assumption that the primary electron beam is unchanged, in intensity, energy, or direction, within the *information depth* (4.37) for Auger-electron emission. This assumption becomes progressively less useful as the primary energy becomes closer to the core-level ionization energy for the relevant *Auger transition* (12.33) or for increasing *angles of incidence* (8.1) of the primary electrons. In such cases, a more advanced theory of electron transport should be used. For example, if the primary electron energy is less than twice the core-level ionization energy, the total Auger-electron current emitted from the sample can be less than that calculated for an unaltered *primary beam* (8.10) alone so that, if the primary beam is assumed to be unaltered, the measured backscattering correction factor would be less than unity and the backscattering fraction is negative. In such cases, the separate classification of the electrons as primary or backscattered becomes progressively less useful.

12.54
backscattering fraction

<AES> ratio of the Auger-electron current arising from ionizations in the sample caused by *backscattered electrons* (12.3) and the Auger-electron current arising directly from the *primary electrons* (12.1)

Note 1 to entry: See *backscattering correction factor* (12.53).

Note 2 to entry: The *AES* (11.1) literature contains many references to “backscattering factor” but the use of this term is ambiguous. In some papers and books, the backscattering factor is the same as the backscattering correction factor, while in other papers and books, the backscattering factor is identified as the backscattering fraction. In practice, this ambiguous usage generally does not cause misunderstanding since the backscattering correction factor (often denoted by R) is equal to unity plus the backscattering fraction (often denoted by r). To avoid misunderstanding, use of the term backscattering factor is deprecated.

Note 3 to entry: In simple theories, evaluations of the backscattering fraction can be based on the assumption that the primary electron beam is unchanged, in intensity, energy, or direction, within the *information depth* (4.37) for Auger-electron emission. This assumption becomes progressively less useful as the primary energy becomes closer to the core-level ionization energy for the relevant *Auger transition* (12.33) or for increasing *angles of incidence* (8.1) of the primary electrons. In such cases, a more advanced theory of electron transport should be used. For example, if the primary electron energy is less than twice the core-level ionization energy, the total Auger-electron current emitted from the sample can be less than that calculated for an unaltered *primary beam* (8.10) alone so that, if the primary beam is assumed to be unaltered, the measured backscattering correction factor would be less than unity and the backscattering fraction is negative. In such cases, the separate classification of the electrons as primary or backscattered becomes progressively less useful.

12.55
differential electron elastic reflection coefficient

<EPES> ratio, per solid angle, of the number of electrons backscattered quasi-elastically from a solid *surface* (3.2) at a given *scattering angle* (8.4) to the number of incident electrons

Note 1 to entry: The differential elastic reflection coefficient for electrons depends on the atomic composition of the surface layer of the solid, on the *differential elastic scattering cross sections* (4.9) of the different atoms for electrons, on the corresponding *inelastic mean free path* (12.41), on the energy of the incident electrons and on the scattering geometry.

12.56

begrenzungs effect

change of the probability of bulk excitation for electrons travelling in condensed matter near a *surface* (3.2) or an *interface* (3.1), arising from the presence of the surface or interface

12.57

bremsstrahlung

<XPS> photon radiation emitted from a material due to the deceleration of incident electrons within that material

Note 1 to entry: The bremsstrahlung radiation has a continuous spectral distribution up to the energy of the incident electrons.

Note 2 to entry: In *XPS* (11.6), the bremsstrahlung from a conventional X-ray source with an Al or Mg anode leads to a continuous photoelectron background. This radiation can also photoionize inner shells, which would be energetically impossible with characteristic Al Kα or Mg Kα X-rays. As a result, *Auger electron* (12.32) features can appear at negative *binding energy scale* (12.73) values and, in addition, the intensities of other Auger electron features can be greater than if the inner shell vacancies had been created only by the *characteristic X-rays* (3.66). The bremsstrahlung-excited Auger electron features can be helpful in determining the various *Auger parameters* (12.80) required to identify *chemical states* (12.23).

12.58

electron spectrometer

device, the essential part of which is an *electron energy analyser* (12.59)

Note 1 to entry: The term electron spectrometer can be used either as a synonym for electron energy analyser or to describe a more complex instrument based on an electron energy analyser and additional electron-optical components. Occasionally, the term is used to describe a complete working system with an energy analyser, possible electron-optical components, an electron detector, excitation sources, vacuum pumps, control electronics, and a data-processing system. The meaning is normally made clear by the context.

12.59

electron energy analyser

device for measuring the number of electrons, or an intensity proportional to that number, as a function of the electron *kinetic energy* (3.35)

Note 1 to entry: See *electron spectrometer* (12.58).

12.60

overpotential

U

<AES> ratio of the electron *beam energy* (8.33) to the *binding energy* (12.16) of a particular shell or sub-shell of an atom

Note 1 to entry: Overpotential values are typically in the range 2 to 200.

12.61

modulation

<AES, differential spectrum> periodic waveform added to the spectrometer *pass energy* (12.63) or applied to the sample in order to generate a display of the *differential spectrum* (12.69)

Note 1 to entry: The amplitude of the modulation should be given as electron volts peak-to-peak, thereby including any relevant geometrical factor of the spectrometer, rather than volts peak-to-peak. The frequency and waveform shape should also be given.

12.62

electron retardation

<AES, XPS> method of measuring the *kinetic energy* (3.35) distribution by retarding the emitted electrons before or within the *electron energy analyser* (12.59)

12.63
pass energy

<AES, ISS, XPS> mean *kinetic energy* (3.35) of the detected particles in the energy-dispersive portion of the energy analyser

12.64
constant ΔE mode
constant analyser energy mode
CAE mode
fixed analyser transmission mode
FAT mode

mode of *electron energy analyser* (12.59) operation that varies the *electron retardation* (12.62) but keeps the *pass energy* (12.63) constant in the energy-dispersive portion of the analyser

Note 1 to entry: This mode is often used in *XPS* (11.6) to maintain a high and constant *energy resolution* (10.24) throughout the spectrum. In this case, the analyser transmission usually falls with increasing *kinetic energy* (3.35) of the analysed electrons.

12.65
constant $\Delta E/E$ mode
constant retardation ratio mode
CRR mode
fixed retardation ratio mode
FRR mode

mode of *electron energy analyser* (12.59) operation that varies the retarding potential so that the *pass energy* (12.63) in the energy-dispersive portion of the analyser is a constant fraction of the original *vacuum level* (12.10) referenced *kinetic energy* (3.35)

Note 1 to entry: This mode is often used in *AES* (11.1) to improve the *signal-to-noise ratio* (3.23) for high-energy emitted electrons at the expense of *energy resolution* (10.24). In this case, the analyser transmission usually rises with increasing kinetic energy of the analysed electrons as a result of the increased energy width accepted.

12.66
photoelectron X-ray satellite peaks

photoelectron peaks in a spectrum resulting from *photoemission* (12.8) induced by characteristic minor X-ray lines associated with the X-ray spectrum of the anode material

EXAMPLE Kα', K$\alpha_{3,4}$, L$\alpha_{5,6}$, and Kβ are all minor X-ray lines.

12.67
X-ray ghost line

<XPS> line in a spectrum due to *photoemission* (12.8) induced by X-ray photons from an impurity in or on the X-ray anode, from the X-ray window, or from certain elements present in the sample

Note 1 to entry: Ghost lines typically appear in dual-anode X-ray sources with Mg and Al coatings where a small fraction of Al X-rays appear when using the Mg source and vice versa. Other common ghost lines appear for oxygen X-rays as the coatings oxidize or copper X-rays from the coating substrate.

12.68
direct spectrum

<AES and XPS> intensity of electrons transmitted and detected by a spectrometer with a dispersing energy analyser, as a function of energy, E

Note 1 to entry: In retarding field energy analysers, which do not have a dispersing element, the direct spectrum can be obtained from the first differential of the collected current with respect to the retarding energy.

Note 2 to entry: By convention, direct spectra in *XPS* (11.6) are often presented in the *constant ΔE mode* (12.64), in which the spectrum approximates the true spectrum, whereas, in *AES* (11.1), spectra are often presented in the *constant $\Delta E/E$ mode* (12.65), in which the spectrum approximates to E times the true spectrum.

12.69
differential spectrum

<AES, XPS> differential of the *direct spectrum* (12.68) with respect to energy, *E*, by an analogue electrode *modulation* (12.61) method or by numerical differentiation of that spectrum

Note 1 to entry: The modulation amplitude in eV or the number of points and the type of differentiating function should be given.

12.70
Auger electron spectrum

plot of the *Auger electron* (12.32) intensity as a function of the electron *kinetic energy* (3.35), usually as part of the energy distribution of detected electrons

Note 1 to entry: When excited by incident electrons, the energy distribution of detected electrons, often measured between 0 eV and 2 500 eV, contains Auger electrons, *backscattered* (primary) *electrons* (12.3) and *secondary electrons* (12.2). The entire distribution is sometimes referred to as an Auger electron spectrum.

Note 2 to entry: The Auger electron spectrum can be presented in either the *direct spectrum* (12.68) or *differential spectrum* (12.69) formats.

12.71
electron energy loss spectrum

energy spectrum of electrons from a nominally monoenergetic source emitted after inelastic interactions with the sample, often exhibiting peaks due to specific inelastic loss processes

Note 1 to entry: See *characteristic electron energy losses* (12.40) and *plasmon* (12.47).

Note 2 to entry: The spectrum obtained using an incident-electron beam of about the same energy as an *AES* (11.1) or *XPS* (11.6) peak approximates to the energy loss spectrum associated with that peak.

Note 3 to entry: The electron energy loss spectrum, measured with an incident-electron beam, is a function of the *beam energy* (8.33), the *angle of incidence* (8.1) of the beam, the *angle of emission* (8.5), and the electronic properties of the sample.

12.72
peak energy

<AES, EELS, ISS, UPS, XPS> energy value corresponding to the intensity maximum in a *direct spectrum* (12.68) or to the intensity minimum (i.e. the negative excursion) for a *differential spectrum* (12.69)

Note 1 to entry: The energy value can relate to the peak envelope for a group of overlapping peaks or to the positions of constituent peaks obtained by *peak synthesis* (3.30).

Note 2 to entry: For the differential spectrum in *AES* (11.1), the *modulation* (12.61), or differentiating amplitude should be given.

Note 3 to entry: The peak energies for the differential spectrum in AES are higher in *kinetic energy* (3.35) than those for the direct spectrum.

12.73
binding energy scale

electron energy axis used to display data in *XPS* (11.6).

Note 1 to entry: *Peak energy* (12.72) on the binding energy scale is not necessarily identical to *binding energy* (12.16) due to *final state* (3.56) effects or uncertainty in *energy referencing* (12.74).

Note 2 to entry: See also *Fermi level referencing* (12.75), *adventitious carbon referencing* (12.77), *internal carbon referencing* (12.78), *gold decoration* (12.79) and *vacuum level referencing* (12.76).

12.74

energy referencing

<AES, XPS> method by which the *charging potential* (8.44) of a sample is determined in order to correct the measured energies so that those energies correspond to a sample with no surface charge

Note 1 to entry: Energy referencing is often conducted using *adventitious carbon referencing* (12.77), using *internal carbon referencing* (12.78) or by *gold decoration* (12.79).

Note 2 to entry: Different charging potentials can occur on different areas or at different depths in a sample, arising, for example, from sample inhomogeneities or non-uniform intensity of the incident *flux* (8.18) of radiation.

12.75

Fermi level referencing

<XPS, UPS> establishing the *binding energy scale* (12.73) for a particular sample by assigning the *kinetic energy* (3.35) corresponding to the *Fermi level* (12.9), as determined by analysis of the sample's *XPS* (11.6) or *UPS* (11.8) spectrum, as the point of zero binding energy

Note 1 to entry: See *vacuum level referencing* (12.76).

12.76

vacuum level referencing

<AES, XPS> method of establishing the *kinetic energy* (3.35) scale in which the zero point corresponds to an electron at rest at the *vacuum level* (12.10)

Note 1 to entry: See *Fermi level referencing* (12.75).

12.77

adventitious carbon referencing

<XPS> determining the *charging potential* (8.44) of a particular sample from a comparison of the experimentally determined C 1s *peak energy* (12.72), arising from adsorbed hydrocarbons on the sample, with a specified energy value

Note 1 to entry: See *energy referencing* (12.74), *Fermi level referencing* (12.75) and *internal carbon referencing* (12.78).

Note 2 to entry: A nominal value of 285,0 eV is often used for the peak energy of the relevant C 1s peak on the *binding energy scale* (12.73), although some analysts prefer specific values in the range 284,6 eV to 285,2 eV, depending on the nature of the substrate. This method does not determine the true charging potential since the true peak energy of the adsorbed hydrocarbons is not known.

Note 3 to entry: Different *sample charging* (8.42) potentials can occur on different areas on the *surface* (3.2), or at different depths, arising, for example, from sample inhomogeneities or non-uniform intensity of the incident-radiation *flux* (8.18).

12.78

internal carbon referencing

<XPS> method by which the *charging potential* (8.44) of a particular sample is determined from a comparison of the experimentally determined C 1s *peak energy* (12.72) arising from a specific carbon group within the sample with a specified energy value for that carbon group

Note 1 to entry: See *energy referencing* (12.74), *adventitious carbon referencing* (12.77) and *Fermi level referencing* (12.75).

Note 2 to entry: A hydrocarbon group within the sample is often used for this purpose.

12.79

gold decoration

<XPS> method whereby a very small quantity of gold, deposited as unconnected islands on an insulator, is used for *energy referencing* (12.74)

Note 1 to entry: See *adventitious carbon referencing* (12.77) and *internal carbon referencing* (12.78).

Note 2 to entry: The gold can be deposited by evaporation or by immersion of the *surface* (3.2) in a solution that produces a colloidal gold deposit.

Note 3 to entry: The *binding energy scale* (12.73) position for the Au $4f_{7/2}$ peak is often taken as 84,0 eV, although measured values of this binding energy for gold deposited on a conducting substrate vary with the average gold island diameter.

12.80
Auger parameter

<XPS> *kinetic energy* (3.35) of a narrow *Auger electron* (12.32) peak in a spectrum minus the kinetic energy of the most intense photoelectron peak from the same element

Note 1 to entry: See *initial-state Auger parameter* (12.81) and *modified Auger parameter* (12.82).

Note 2 to entry: The value of the Auger parameter depends on the energy of the X-rays, which therefore shall be specified.

Note 3 to entry: The Auger parameter is sometimes called the *final state* (3.56) Auger parameter.

Note 4 to entry: The Auger parameter is useful for separating *chemical states* (12.23) for samples in which charging causes uncertainty in the *binding energy scale* (12.73) measurement or in which the binding energy shift is inadequate to identify the chemical state.

Note 5 to entry: The Auger parameter is useful for evaluating the *relaxation energy* (3.59) of the ionized matrix atom associated with the generation of a core *hole* (3.61) for those *Auger transitions* (12.33) between core levels which have similar *chemical shifts* (12.18).

12.81
initial-state Auger parameter

<XPS> β, where $\beta = 3E_B + E_K$ and where E_B and E_K are, respectively, the *binding energy scale* (12.73) position of a photoelectron peak and the *Fermi level* (12.9) referenced *kinetic energy* (3.35) of an *Auger electron* (12.32) peak, each involving the same initial core level of the same element

Note 1 to entry: See *Auger parameter* (12.80) and *modified Auger parameter* (12.82).

Note 2 to entry: The initial-state Auger parameter is useful for evaluating the change in the atomic core potential contribution to changes in binding energy between two environments, providing the *Auger transition* (12.33) is between core levels that have similar binding energy shifts.

Note 3 to entry: This parameter has no relation to the *asymmetry parameter* (12.28) which is also given the symbol β.

12.82
modified Auger parameter

<XPS> sum of the *Fermi level* (12.9) referenced *kinetic energy* (3.35) of a narrow *Auger electron* (12.32) peak in the spectrum and the *binding energy scale* (12.73) position of the most intense photoelectron peak from the same element

Note 1 to entry: See *Auger parameter* (12.80) and *initial-state Auger parameter* (12.81).

Note 2 to entry: The modified Auger parameter is the sum of the Auger parameter and the energy of the X-rays responsible for the measured photoelectron peak. Unlike the Auger parameter, it does not depend on the energy of the X-rays.

12.83
chemical-state plot
Wagner plot

<XPS> plot of the measured *kinetic energy* (3.35) of a sharp *Auger electron* (12.32) peak versus the *binding energy scale* (12.73) position of a photoelectron peak for the same element

Note 1 to entry: Plots are usually made for a given element that can exist in different *chemical states* (12.23). Such plots are helpful in defining the state for an unknown sample where measurements of the binding energy alone are inadequate.

Note 2 to entry: The binding energy is usually plotted on the abscissa with values decreasing towards the right.

12.84
photoelectron X-ray satellite subtraction

removal of *photoelectron X-ray satellite peaks* (12.66) from a spectrum

Note 1 to entry: For unmonochromated Al and Mg X-rays, the satellites usually removed are K$\alpha_{3,4}$ and K$\alpha_{5,6}$. More sophisticated subtraction methods also remove the Kα_2, Kα', and Kβ satellites.

12.85
inelastic electron scattering background subtraction

<AES, XPS> process for subtracting a chosen *inelastic scattering* (4.2) background from the measured spectrum

Note 1 to entry: See *inelastic background* (12.46), *Shirley background* (12.86), and *Tougaard background* (12.88).

Note 2 to entry: For *AES* (11.1) and *XPS* (11.6), the inelastic background associated with a particular *Auger electron* (12.32) or photoelectron peak has been approximated by a measured *electron energy loss spectrum* (12.71) for which the incident-electron energy is close to the energy of the peak. The Tougaard background is also used. A simpler, but less accurate, inelastic background function is the Shirley background. Simple linear backgrounds have also been used, but these are much less accurate except for the XPS analysis of insulators.

12.86
Shirley background

<AES, XPS> background calculated to fit the measured spectrum at points at higher and lower *kinetic energy* (3.35) than the peak or peaks of interest such that the background contribution at a given kinetic energy is in a fixed proportion to the total *peak area* (3.16) above that background for higher kinetic energies

Note 1 to entry: See *Tougaard background* (12.88).

Note 2 to entry: The fitting to the background can be made by averaging over a given number of energy channels.

12.87
Sickafus background

<AES, XPS> single-term power law background designed to describe the intensity of the *secondary electron* (12.2) cascade as a function of electron emission *kinetic energy* (3.35)

Note 1 to entry: The measured secondary-electron cascade, for correction application of the Sickafus background, should be the experimentally observed spectrum corrected for the *spectrometer response function* (7.13) of the measuring instrument.

Note 2 to entry: The spectrum shape, for a Sickafus background $B_s(E)$, is given by

$$B_s(E) \propto E^{-m}$$

where E is the electron emission kinetic energy and m is a number in the range 1 to 2.

12.88
Tougaard background

<AES, XPS> intensity distribution obtained from a model for the differential *inelastic scattering cross section* (12.39) with respect to *energy loss* (4.3) and the three-dimensional distribution of the emitting atoms in the surface region

Note 1 to entry: See *Shirley background* (12.86).

Note 2 to entry: A number of classes of atomic distributions can be used together with different differential inelastic scattering cross sections. The atomic distribution and the inelastic scattering cross section should be specified.

Note 3 to entry: The Tougaard background is usually calculated to match the measured spectrum over a wide energy range that excludes the peak region and the spectral region extending to approximately 50 eV less *kinetic energy* (3.35) than the peaks of interest. The measured spectrum should be corrected for the *spectrometer response function* (7.13) of the measuring instrument before calculation of the Tougaard background.

12.89
partial intensity

<AES, EPES, REELS, XPS> total number of electrons in an electron spectrum, originating from a given *Auger transition* (12.33) or photoelectric transition, or associated with *primary electrons* (12.1) backscattered from a *surface* (3.2), per unit of excitation or of backscattering, that reach the detector after participating in a given number of inelastic interactions of a given type

Note 1 to entry: The zero-order partial intensity is the number of electrons, originating from the peak of interest in the spectrum, that reach the detector without any inelastic interaction in the solid or the vacuum. This intensity is the area under the photoelectron or *Auger electron* (12.32) peak of interest or under the peak corresponding to the elastically *backscattered electrons* (12.3).

Note 2 to entry: In a solid, an electron can experience different types of *inelastic scattering* (4.2), such as those associated with volume or surface effects. The inclusion or exclusion of specific types of inelastic scattering in calculations of partial intensities should be stated.

Note 3 to entry: The partial intensity is a dimensionless number.

12.90
reduced partial intensity

<AES, EPES, REELS, XPS> ratio of the *partial intensity* (12.89) to the zero-order partial intensity

Note 1 to entry: The reduced partial intensity is a dimensionless number.

12.91
average matrix relative sensitivity factor
AMRSF

<AES, XPS> coefficient, proportional to the intensity, calculated for an element in an average matrix, by which the measured intensity for that element is divided in calculations to yield the atomic concentration or atomic fraction of the element present in the sample

Note 1 to entry: See sensitivity factor, *elemental relative sensitivity factor* (12.92) and *pure element relative sensitivity factor* (12.93).

Note 2 to entry: The choice of atomic concentration or atomic fraction should be made clear.

Note 3 to entry: The type of sensitivity factor utilized should be appropriate for the formulae used in the quantification process and for the type of sample analysed, for example homogeneous samples or segregated layers.

Note 4 to entry: The source of sensitivity factors should be given. *Matrix factors* (3.11) are taken to be unity for average matrix relative sensitivity factors.

Note 5 to entry: Sensitivity factors depend on parameters of the excitation source, the spectrometer, and the orientation of the sample to these parts of the instrument. The numerical values of the sensitivity factors can also depend on the method used to measure the peak intensities.

12.92
elemental relative sensitivity factor

<AES, XPS> coefficient proportional to the *absolute elemental sensitivity factor* (3.12), where the constant of proportionality is chosen such that the value for a selected element and transition is unity

Note 1 to entry: Elements and transitions commonly used are C 1s or F 1s for *XPS* (11.6) and Ag $M_{4,5}VV$ for *AES* (11.1).

Note 2 to entry: The type of sensitivity factor used should be appropriate for the type of sample analysed, for example homogeneous samples or segregated layers.

Note 3 to entry: The source of sensitivity factors should be given to ensure that the correct *matrix factors* (3.11) or other parameters are used.

Note 4 to entry: Sensitivity factors depend on parameters of the excitation source, the spectrometer, and the orientation of the sample to these parts of the instrument. Sensitivity factors also depend on the matrix being analysed, and in *SIMS* (19.1) this has a dominating influence.

12.93
pure element relative sensitivity factor
PERSF

<AES, XPS> coefficient, proportional to the intensity measured for a pure sample of an element, by which the measured intensity for that element is divided in calculations to yield the atomic concentration or atomic fraction of the element present in the sample

Note 1 to entry: See sensitivity factor, *elemental relative sensitivity factor* (12.92), and *average matrix relative sensitivity factor* (12.91).

Note 2 to entry: The choice of atomic concentration or atomic fraction should be made clear.

Note 3 to entry: The type of sensitivity factor used should be appropriate for the formulae used in the quantification process and for the type of sample analysed, for example homogeneous samples or segregated layers.

Note 4 to entry: The source of sensitivity factors should be given to ensure that the correct *matrix factors* (3.11) or other parameters are used. Matrix factors are significant and should be used with pure-element relative sensitivity factors.

Note 5 to entry: Sensitivity factors depend on parameters of the excitation source, the spectrometer, and the orientation of the sample to these parts of the instrument. The numerical values of the sensitivity factors can also depend on the method used to measure the peak intensities.

12.94
valence-band spectrum

<XPS> photoelectron energy distribution arising from excitation of electrons from the valence band of the sample material

13 Terms related to X-ray fluorescence, reflection and scattering methods

13.1
X-ray absorption fine structure spectroscopy
XAFS

method to measure the absorption of X-rays at energies near and above (typically several hundred eV higher) an absorption edge, over which fine structure (modulation of the X-ray absorption coefficient) can be detected

Note 1 to entry: XAFS includes both *EXAFS* (13.2) and *XANES* (13.4). It involves transitions from a core-level to an unoccupied orbital or band and mainly reflects the local atomic structure and bonding (EXAFS) and the density of the unoccupied electronic states (XANES).

Note 2 to entry: XAFS, XANES, and NEXAFS measurements usually start some 10 eV before the core-level *binding energy* (12.16) (the absorption edge) of the emitting atoms because in many cases pre-edge features are used to identify chemical bonds, e.g. pi* resonances (excitation into lowest unoccupied molecular orbitals) in C K-edge spectra of polymer samples.

Note 3 to entry: Usefully sharp absorption edges are commonly observed in X-ray absorption spectra although broader increases can be observed for some inner-shell excitations with short lifetimes.

13.2
extended X-ray absorption fine structure spectroscopy
EXAFS

XAFS (13.1) in the energy region from the core-level edge to an energy several hundred eV higher

Note 1 to entry: Extended X-ray absorption fine structure results mainly from single scattering of the photoelectron from surrounding atoms and is exhibited as oscillations in the absorption cross section with increasing photon energy. Analysis of the oscillations provides information, through bond lengths, on the local chemical environment of the emitting atom.

13.3
surface extended X-ray absorption fine structure spectroscopy
SEXAFS

XAFS (13.1) in which, instead of measuring the X-ray absorption, the *Auger-electron* (12.32) or *secondary electron* (12.2), emission arising from that absorption is measured

Note 1 to entry: The detection of Auger or secondary electrons provides greater surface sensitivity than generally found with extended X-ray absorption fine structure measurements.

13.4
X-ray absorption near-edge spectroscopy
XANES

near-edge X-ray absorption fine structure spectroscopy

NEXAFS

XAFS (13.1) in the energy region near (within approximately 100 eV) an absorption edge

Note 1 to entry: XANES results from interference in multiple scattering of low-energy photoelectrons by surrounding atoms. It provides information on the local coordination environment, oxidation state, molecular orbitals, hybridization, and band structure (unoccupied electronic states).

Note 2 to entry: XAFS, XANES, and NEXAFS measurements usually start some 10 eV before the core-level *binding energy* (12.16) (the absorption edge) of the emitting atoms, because in many cases pre-edge features are used to identify chemical bonds, e.g pi* resonances (excitation into lowest unoccupied molecular orbitals) in C K-edge spectra of polymer samples.

Note 3 to entry: Usefully sharp absorption edges are commonly observed in X-ray absorption spectra although broader increases can be observed for some inner-shell excitations with short lifetimes.

13.5
small-angle X-ray scattering
SAXS

method in which the elastically scattered intensity of X-rays is measured for small-angle deflections

Note 1 to entry: The scattering is typically measured in the angular range up to 5°. This provides structural information about inhomogeneities in materials with characteristic lengths typically ranging from 1 nm to 100 nm. Under certain conditions the limit of 100 nm can be significantly extended.

Note 2 to entry: Wide-angle X-ray scattering (WAXS) is an analogous technique, similar to X-ray crystallography, in which scattering at larger angles, which is sensitive to periodicity on smaller length scales, is measured.

13.6
grazing incidence small-angle X-ray scattering
GISAXS

method in which the elastically scattered intensity of X-rays from a reflecting surface is measured for small *glancing angle* (8.2) deflections at *grazing incidence* (8.3)

Note 1 to entry: The glancing angle depends on photon energy and material and is typically < 2°. GISAXS provides structural information of the surface or for particles on the surface for lengths scales between several nm and several hundred nm.

13.7
X-ray reflectometry
XRR

method of analysing *surface* (3.2) and *interface* (3.1) roughness and density, layer thickness of thin layers, and the electron density profile by reflecting X-rays from a flat sample and analysing the reflected intensity as a function of angle

Note 1 to entry: See *specular XRR* (13.8).

Note 2 to entry: Monochromatic X-rays of low divergence are required. Many layers can be modelled with thicknesses between ~1 nm and a few µm and (subject to conditions) fitted to the data. The surface must be flat over the *beam footprint* (14.6) of typically 10 mm to 40 mm.

13.8
specular XRR

mode of *XRR* (13.7) in which the angle between the detected beam and the sample surface, and the incident beam and the sample surface, are equal

Note 1 to entry: See *off-specular XRR* (13.9).

Note 2 to entry: Specular XRR is the customary mode for XRR and is often meant when the term XRR is used.

Note 3 to entry: In this case, the *scattering angle* (8.4) 2θ is twice the *glancing angle* (8.2), ω. The detected, scattered X-ray intensity is measured as a function of either ω or 2θ or the *scattering vector* (14.2), $\boldsymbol{q}_z$. The intensity data are usually presented as a function of $\boldsymbol{q}_z$ or ω.

13.9
off-specular XRR
diffuse XRR

XRR (13.7) in which significant scattered intensity arises from imperfections of the specimen, the scattered intensity falling outside the specular condition

Note 1 to entry: See *specular XRR* (13.8).

Note 2 to entry: Imperfections generating diffuse XRR include *surface* (3.2) and *interface* (3.1) roughnesses, film defects, and inhomogeneities. By modelling, quantitative estimates can be made of these.

13.10
X-ray emission spectroscopy
XES

method in which the X-ray fluorescent intensities from a surface are measured with high energy *resolving power* (10.5) to identify changes due to the chemical environments of elements

13.11
total reflection X-ray fluorescence
TXRF

method in which an X-ray spectrometer is used to measure the energy distribution of *fluorescence* (3.64) X-rays emitted from a *surface* (3.2) irradiated by primary X-rays under the condition of total reflection

Note 1 to entry: See *critical angle* (14.5).

13.12
grazing incidence X-ray fluorescence
GIXRF

method in which X-ray fluorescence intensities are measured as a function of the *glancing angle* (8.2) of incident X-rays

Note 1 to entry: For flat surfaces with low surface roughness an X-ray standing wave field modifies the excitation beam intensity as a function of the *glancing angle* (8.2).

Note 2 to entry: The angle of incidence covers the region below and above the *critical angle* (14.5) of total external reflection of the substrate.

13.13
grazing emission X-ray fluorescence
GEXRF
method in which X-ray fluorescence intensities are measured as a function of the *take-off angle* (8.7) of *grazing exit* (8.6) X-rays

Note 1 to entry: In contrast to *GIXRF* (13.12), the X-ray incidence can be perpendicular to the surface so that the *beam footprint* (14.6) is not larger than the beam width.

Note 2 to entry: If a detector with spatial resolution is used, an angle-scan free operation without mechanical motion is possible.

14 Terms related to X-ray fluorescence, reflection and scattering analysis

14.1
dispersion plane
<XRR> plane containing the source, detector, incident, and specularly reflected X–ray beams

14.2
scattering vector
q
<XRR, SAXS, GISAXS> vector in reciprocal space giving the difference between the scattered and incident wave vectors

Note 1 to entry: See *wave vector* (14.3).

14.3
wave vector
k
<XRR, SAXS, GISAXS> vector in reciprocal space describing the direction of propagation of X-rays and equal in magnitude to $2\pi/\lambda$, where λ is the wavelength of the X-rays

Note 1 to entry: See *scattering vector* (14.2).

14.4
absorption length
distance over which the transmitted X-ray intensity falls by 1/e, where e is the base of the natural logarithm

14.5
critical angle
<XRR, TXRF, GIXRF> angle between the incident beam and the specimen surface at which the reflectivity is at the first point of inflexion

Note 1 to entry: In practical cases, the critical angle is often taken as the angle at which the reflected intensity has fallen to 50 % of that in the total external reflection condition. The error here is generally small.

Note 2 to entry: The critical angle for a given specimen material or structure can be found by using simulation software, or by calculation from the formula $\theta_c \approx (2\delta)^{0,5}$, where $1-\delta$ is the real part of the complex X-ray refractive index given by $n = 1 - \delta - i\beta$.

14.6
beam footprint
<XRR, TXRF, GIXRF> area on the specimen irradiated by the X-rays

Note 1 to entry: In typical commercial equipment, the beam width is about 200 µm, so for example at 0,3° *glancing angle* (8.2), the beam footprint is 38 mm long; at 1°, it is 11,5 mm. For 100 µm incident beam width, these values are halved.

Note 2 to entry: The beam footprint along the beam direction can be reduced by the use of a suitable knife-edge diaphragm mounted in a plane that is normal to the sample surface and whose normal, in turn, aligns with the beam azimuth. The knife-edge is parallel to, and adjusted to be close to, the surface at the point where the X-ray beam centre strikes the sample surface. This closeness limits the footprint size but also reduces the measured *signal intensity* (3.17).

14.7
beam spill-off
<XRR> fraction of the incident X-ray beam missing the specimen

14.8
delayed onset
X-ray energy, in an X-ray absorption spectrum, at which there is a significant increase of absorption and for which the increased absorption occurs at a higher energy than a core-level *binding energy* (12.16)

Note 1 to entry: For many elements, there is a significant increase of absorption when the X-ray energy is equal to the electron-binding energy for a sub-shell. A delayed onset occurs for some elements and sub-shells when the corresponding increase of absorption occurs, instead, at an energy larger than the sub-shell binding energy.

14.9
jump ratio
ratio of the X-ray absorption coefficient at an energy just above an absorption edge to that at an energy just below the edge

Note 1 to entry: X-ray absorption spectra can have complex shapes for X-ray energies in the vicinity of photoionization thresholds, and a well-defined edge is not always observed at the threshold.

15 Terms related to glow discharge methods

15.1
glow discharge spectrometry
GDS
method in which a spectrometer is used to measure relevant intensities emitted from a *glow discharge* (16.2) generated at a *surface* (3.2)

Note 1 to entry: This is a general term that encompasses *GDOES* (15.3) and *GDMS* (15.2).

15.2
glow discharge mass spectrometry
GDMS
method in which a mass spectrometer is used to measure *m/z* (20.1) and abundance of ions from a *glow discharge* (16.2) generated at a *surface* (3.2)

15.3
glow discharge optical emission spectrometry
GDOES
method in which an optical emission spectrometer is used to measure the wavelength and intensity of light emitted from a *glow discharge* (16.2) generated at a *surface* (3.2)

16 Terms related to glow discharge analysis

16.1
plasma
<GDS> gas consisting of ions, electrons, and neutral particles

Note 1 to entry: Gases are weakly ionized in *glow discharge* (16.2).

16.2
glow discharge

phenomenon that results from the passage of electrical current through a gas and that is characterized by emission of light, a low current density (about 0,01 A/m^2 to 1 000 A/m^2), and a potential that is above the ionization potential of the gas but below the sparking potential

Note 1 to entry: In glow discharge surface-analytical instruments, sample material is introduced into the gaseous discharge via bombardment of the *surface* (3.2) by positive ions and energetic neutral species. Sputtered atoms are then excited and ionized by collisions in the discharge.

Note 2 to entry: Analytical glow discharge devices are usually operated in argon at a pressure in the range 10 Pa to 2 000 Pa.

16.3
abnormal glow discharge

<GDS> *glow discharge* (16.2) operated in a current/voltage regime in which an increase in current is accompanied by an increase in voltage

Note 1 to entry: See *normal glow discharge* (16.5).

Note 2 to entry: Glow discharge devices used for surface chemical analysis are usually operated in the abnormal mode, rather than the normal mode. This is because abnormal operation provides *sputtering* (9.3) of the entire exposed *surface* (3.2) of the sample, as well as increased signal intensities.

16.4
boosted glow discharge

<GDS> *glow discharge* (16.2) sustained by a secondary means of coupling energy into the *plasma* (16.1) in addition to the primary means, sometimes providing enhanced analytical signals

Note 1 to entry: Forms of boosting the glow discharge include the use of microwave and rf fields (not to be confused with unboosted rf glow discharge, in which rf excitation is the only power source), as well as the injection of extra plasma electrons by means of filaments or other electron sources.

16.5
normal glow discharge

<GDS> *glow discharge* (16.2) operated in a current/voltage regime in which an increase in current is accompanied by little or no detectable change in voltage

Note 1 to entry: See *abnormal glow discharge* (16.3).

Note 2 to entry: Glow discharge devices used for surface chemical analysis are not usually operated in the normal mode. This is because a portion of the exposed sample *surface* (3.2) remains unsputtered and signal intensities can be unacceptably weak. Such devices are usually operated in the abnormal mode.

16.6
pulsed glow discharge

<GDS> *glow discharge* (16.2) in which one or more of the discharge operating parameters are intentionally varied in time in order to provide improved analytical performance

Note 1 to entry: The most common pulsed glow discharge involves *modulation* (12.61), in accordance with a square-wave or similar function, of the electrical power maintaining the *plasma* (16.1). However, other forms of pulsed glow discharge are possible.

Note 2 to entry: Both pulsed-DC and pulsed-rf glow discharges have been devised.

16.7

jet-assisted glow discharge source

jet-enhanced glow discharge source

<GDS> *glow discharge* (16.2) device incorporating a means of directing high-velocity jets of plasma-support gas directly towards the sample *surface* (3.2), intended to provide enhanced analytical signals

Note 1 to entry: This form of glow discharge device has been used predominantly for glow discharge atomic absorption spectrophotometry. The jets enhance atomic absorption by aiding the transport of sputtered material from the sample surface into the region of the *negative glow* (16.20) in which light absorption is measured.

Note 2 to entry: Jet-enhanced glow discharge devices find little use for *depth profiling* (3.34) because the craters formed on the sample surface are not usually flat.

16.8

anode

<GDS, DC operation> more positively charged electrode in a *glow discharge* (16.2) device

Note 1 to entry: See *cathode* (16.10) <GDS, DC operation>.

16.9

anode

<GDS, rf operation> electrode that is more positively charged over a large fraction of the rf cycle in a radio-frequency-powered *glow discharge* (16.2) device

Note 1 to entry: See *cathode* (16.11).

Note 2 to entry: The rf power applied to a typical rf glow discharge device that is used for surface chemical analysis is sinusoidal and bipolar, with a time-averaged electric potential of zero relative to ground potential. The reason that the anode is not more positively charged over the entire rf cycle is that the magnitude of the *DC bias* (16.16) is usually slightly less than one-half of the applied rf peak-to-peak potential.

Note 3 to entry: The precise fraction of the rf cycle over which the anode is more positively charged depends upon the source geometry and other factors.

16.10

cathode

<GDS, DC operation> more negatively charged electrode in a *glow discharge* (16.2) device

Note 1 to entry: See *anode* (16.8).

16.11

cathode

<GDS, rf operation> electrode that is more negatively charged over a large fraction of the rf cycle in a radio-frequency-powered *glow discharge* (16.2) device

Note 1 to entry: See *anode* (16.9).

Note 2 to entry: The rf power applied to a typical rf glow discharge device that is used for surface chemical analysis is sinusoidal and bipolar, with a time-averaged electric potential of zero relative to ground potential. The reason that the cathode is not more negatively charged over the entire rf cycle is that the magnitude of the *DC bias* (16.16) is usually slightly less than one-half of the applied rf peak-to-peak potential.

Note 3 to entry: The precise fraction of the rf cycle over which the cathode is more negatively charged depends upon the source geometry and other factors.

16.12
secondary cathode

<GDS> electrically conductive mask, containing an aperture, used to allow *sputtering* (9.3) of an electrically non-conductive sample *surface* (3.2) in a direct-current *glow discharge* (16.2) device

Note 1 to entry: The secondary cathode is placed in direct contact with the insulating-sample surface, and both the secondary cathode and the surface of the sample within the aperture are exposed to the glow discharge. The secondary cathode is held at *cathode* (16.10) potential, resulting in sputtering of its surface. Some of the material sputtered from the secondary cathode is deposited on the insulating-sample surface within the aperture, causing that surface to become electrically conductive. This results in sputtering of the insulating sample.

Note 2 to entry: When electrically non-conductive samples shall be analysed, the secondary-cathode technique provides a useful alternative to an rf glow discharge.

16.13
sheath
electrode sheath

<GDS> region of *plasma* (16.1) adjacent to an electrode *surface* (3.2), characterized by a *plasma potential* (16.18) that changes with distance from the electrode, being equivalent to the electrode potential at the electrode surface and approaching the plasma potential of the surrounding plasma at sufficiently large distances

Note 1 to entry: These terms are usually applied to an rf *glow discharge* (16.2), though they can also be applied to a DC glow discharge.

16.14
sheath potential

<GDS> electric potential drop across a *sheath* (16.13)

Note 1 to entry: In surface chemical analysis, this term is usually applied to an rf *glow discharge* (16.2), rather than to a DC glow discharge, for which terms such as *cathode fall* (16.15) are much more commonly employed. However, sheath potential can also be applied to a DC glow discharge.

16.15
cathode fall
fall potential

<GDS> electric potential difference between the *cathode* (16.10) surface and the *negative glow* (16.20)

Note 1 to entry: In direct-current *glow discharge spectrometry* (15.1) typically used for surface chemical analysis, the cathode fall is usually in the range 200 V to 2 000 V, with the cathode surface being more negative. In an rf *glow discharge* (16.2), the cathode fall is time-varying, with a peak-to-peak value normally in the range 500 V to 2 000 V.

16.16
DC bias
DC offset
self bias

<GDS, rf operation> time-averaged electric potential, relative to ground, developed on the *surface* (3.2) of the electrode to which the rf power is applied

Note 1 to entry: The DC bias arises as a result of the very different mobilities of the *plasma* (16.1) electrons and the positively charged plasma ions.

Note 2 to entry: The DC bias effectively limits *sputtering* (9.3) to the sample surface, preventing sputtering of other surfaces in contact with the plasma.

Note 3 to entry: For a properly designed rf *glow discharge* (16.2) device used for surface chemical analysis, the magnitude of the DC bias is slightly less than one-half of the applied rf peak-to-peak potential difference.

16.17
floating potential
<GDS> electric potential that develops on an isolated substrate immersed in a *plasma* (16.1)

Note 1 to entry: An isolated substrate cannot conduct charge to other parts of the instrument. Therefore, averaged over time, the *fluxes* (8.18) of electrons and positively charged ions to its *surface* (3.2) shall be equal. Given that electrons are much more mobile than positively charged ions, equal fluxes arise when the floating potential is typically a few volts more negative than the *plasma potential* (16.18).

16.18
plasma potential
<GDS> electric potential of *plasma* (16.1) relative to an appropriate reference such as ground potential

Note 1 to entry: The plasma potential of direct current *glow discharge* (16.2) varies with location in the plasma. The plasma potential of an rf glow discharge varies with both location in the plasma and time, according to the phase of the rf excitation.

16.19
anode glow
<GDS> thin luminous region of a *glow discharge* (16.2) immediately adjacent to the *anode* (16.8)

Note 1 to entry: See *cathode layer* (16.23), *negative glow* (16.20), and *positive column* (16.21).

Note 2 to entry: The anode glow may not be noticeable in a glow discharge used for surface chemical analysis.

16.20
negative glow
<GDS> region of a *glow discharge* (16.2) from which most light is emitted and from which analytical signals for surface chemical analysis are usually derived

Note 1 to entry: See *cathode layer* (16.23), *positive column* (16.21), and *anode glow* (16.19).

16.21
positive column
<GDS> diffuse, luminous region of *glow discharge* (16.2) between the *Faraday* (16.28) and *anode dark spaces* (16.25)

Note 1 to entry: See *cathode layer* (16.23), *negative glow* (16.20), and *anode glow* (16.19).

Note 2 to entry: The positive column is usually absent in glow discharge devices operated for surface chemical analysis, owing to the gas pressure and the small separation between the electrodes.

16.22
afterglow
<GDS> luminescence of the decaying *plasma* (16.1) present in a *glow discharge* (16.2) device after complete cessation of the sustaining discharge power

16.23
cathode layer
<GDS> thin luminous region of *glow discharge* (16.2) between the *Aston dark space* (16.26) and the *cathode dark space* (16.27)

Note 1 to entry: See *negative glow* (16.20), *positive column* (16.21), and *anode glow* (16.19).

Note 2 to entry: The cathode layer may not be noticeable in a glow discharge used for surface chemical analysis.

16.24
dark space
<GDS> region of a *glow discharge* (16.2) that emits little light compared to the surrounding regions, thereby appearing dark to the human eye

16.25
anode dark space

<GDS> *dark space* (16.24) between the *positive column* (16.21) and the *anode glow* (16.19) in a *glow discharge* (16.2)

Note 1 to entry: See *Aston dark space* (16.26), *cathode dark space* (16.27), and *Faraday dark space* (16.28).

16.26
Aston dark space

<GDS> very thin *dark space* (16.24) immediately adjacent to the *cathode* (16.10) in a *glow discharge* (16.2)

Note 1 to entry: See *cathode dark space* (16.27), *Faraday dark space* (16.28), and *anode dark space* (16.25).

Note 2 to entry: In *glow discharge spectrometry* (15.1) used for surface chemical analysis, the Aston dark space is often not noticeable.

16.27
cathode dark space

<GDS> *dark space* (16.24) between the *cathode layer* (16.23) and the *negative glow* (16.20) in a *glow discharge* (16.2)

Note 1 to entry: See *Aston dark space* (16.26), *Faraday dark space* (16.28), and *anode dark space* (16.25).

Note 2 to entry: In *glow discharge spectrometry* (15.1) used for surface chemical analysis, the cathode dark space usually appears to occupy all of the space between the *cathode* (16.10) surface and the negative glow.

Note 3 to entry: In DC glow discharge spectrometry, the cathode dark space is characterized by a large positive space charge and a strong electric field. This situation also occurs in an rf glow discharge over a large majority of the rf cycle. As a result, efficient acceleration of charged particles occurs in the cathode dark space.

16.28
Faraday dark space

<GDS> *dark space* (16.24) between the *negative glow* (16.20) and the *positive column* (16.21) in a *glow discharge* (16.2)

Note 1 to entry: See *Aston dark space* (16.26), *cathode dark space* (16.27), and *anode dark space* (16.25).

16.29
electron impact ionization

<GDS> ionization resulting from collision of an atom, molecule, or ion with an electron

Note 1 to entry: For example, $M + e^- \rightarrow M^+ + 2e^-$, where M^+ is a transition metal ion.

Note 2 to entry: Electron impact ionization is possible only if the *kinetic energy* (3.35) of the relative motion of the collision partners exceeds the difference between

a) the product of the magnitude of the electronic charge and the ionization potential of the particle to be ionized, and

b) the potential energy of that particle prior to collision.

Note 3 to entry: In a *glow discharge* (16.2) used for surface chemical analysis, electron impact ionization usually accounts for a large fraction of the total ionization occurring in the *plasma* (16.1). Therefore, it is a very important physical mechanism for *glow discharge mass spectrometry* (15.2).

16.30
Penning ionization

<GDS> ionization resulting from collision with an atom that is in an electronically *excited state* (3.53)

Note 1 to entry: For example, $Ar^{ms} + M \rightarrow Ar + M^{+} + e^-$, where Ar^{ms} is a metastable Ar atom and M is a transition metal.

Note 2 to entry: Penning ionization is possible only if the sum of the excitation potential of the excited-state atom and the *kinetic energy* (3.35) of the relative motion of the collision partners exceeds the difference between

a) the product of the magnitude of the electronic charge and the ionization potential of the particle that is to be ionized, and

b) the potential energy of that particle prior to collision.

Note 3 to entry: The probability of Penning ionization is directly related to the excited-state lifetime of the excited-state collision partner. For this reason, Penning ionization usually occurs through collisions with metastable species.

Note 4 to entry: In a *glow discharge* (16.2) used for surface chemical analysis, Penning ionization is usually an important ionization mechanism, owing to the fact that the metastable energy levels of Ar, the discharge gas most commonly employed, lie sufficiently above the ionization potentials of most atomic *analytes* (3.4).

16.31
thermalized electrons
<GDS> electrons which, following collisions in the *plasma* (16.1), have an equilibrium energy distribution corresponding to the plasma temperature

16.32
primary electron
<GDS> electron that enters the *negative glow* (16.20) region from the *cathode dark space* (16.27), having been accelerated by the strong electric field within the cathode dark space, thereby having a *kinetic energy* (3.35) that is among the highest of the kinetic energies of any electrons present within the plasma

Note 1 to entry: See *secondary electron* (16.33).

Note 2 to entry: This term is defined differently for *AES* (11.1), electron probe microanalysis, and SEM.

16.33
secondary electron
<GDS> electron with a *kinetic energy* (3.35) intermediate between the kinetic energies of primary and *thermalized electrons* (16.31), produced through ionization or incomplete thermalization of *primary electrons* (16.32)

Note 1 to entry: This term is defined differently for general use in 12.2. Both definitions are used in *GDS* (15.1), depending on the context.

16.34
electron impact excitation
<GDS> electronic excitation of an atom, molecule or ion resulting from collision with an electron

Note 1 to entry: For example, $M + e^- \rightarrow M^* + e^-$, where M^* is a transition metal in an electronically *excited state* (3.53).

Note 2 to entry: In a *glow discharge* (16.2) used for surface chemical analysis, electron-impact excitation is believed to account for most of the electronic excitations. Therefore, it is a very important physical mechanism for *glow discharge optical emission spectrometry* (15.3).

16.35
charge transfer
charge exchange
<GDS> transfer of charge from an atom, molecule or ion to another atom, molecule or ion

16.36

asymmetric charge transfer

asymmetric charge exchange

<GDS> *charge transfer* (16.35) between an atom, molecule or ion and another atom, molecule or ion of a different *chemical species* (3.5)

Note 1 to entry: For example, $Ar^+ + M \rightarrow Ar + M^{+*}$, where M is often a transition metal in *GDS* (15.1) applications and M^{+*} is in an electronically excited, ionic state.

Note 2 to entry: Generally, asymmetric charge transfer is less efficient than *symmetric charge transfer* (16.37), owing to the effects of energy overlap and quantum-mechanical considerations on reaction *cross sections* (4.7).

16.37

symmetric charge transfer

symmetric charge exchange

<GDS> *charge transfer* (16.35) between an atom, molecule or ion and another atom, molecule or ion of the same *chemical species* (3.5)

Note 1 to entry: For example, $Ar^+ + Ar \rightarrow Ar + Ar^+$. This reaction is believed to be an efficient mechanism in the *cathode dark space* (16.27) of an analytical *glow discharge* (16.2), resulting in a large population of fast Ar atoms directed toward the sample *surface* (3.2). These fast Ar atoms can contribute significantly to sample *sputtering* (9.3).

16.38

recombination

ion-electron recombination

<GDS> addition of an electron to an ion with a net positive charge, resulting in a net charge that is one elementary charge unit more negative

Note 1 to entry: Energy and momentum cannot be simultaneously conserved in an ion-electron recombination process that involves the collision of only an ion and an electron and that releases no additional particles. For this reason, recombination proceeds only through the involvement of a third collision partner, such as another electron or a *surface* (3.2), or through the release of a photon.

16.39

radiative recombination

<GDS> *ion-electron recombination* (16.38) involving the release of a photon

16.40

abundance sensitivity

<GDMS> ratio of the maximum ion current recorded at a mass m to the ion current arising from the same species recorded at an adjacent mass ($m \pm 1$)

[SOURCE: IUPAC]

16.41

ion beam ratio

<GDMS> intensity of the *analyte* (3.4) ion divided by the intensity of the matrix ion, both corrected for isotopic abundance

16.42

emission yield

<GDOES> quotient of the time-integrated optical emission signal minus the signal background at a specified wavelength by the mass of the emitting element sputtered in the time interval of interest

16.43

self-absorption

<GDOES> absorption of emitted light by a species, identical to the emitting species, positioned between the emitting species, and the optical detector

Note 1 to entry: Self-absorption results in nonlinear calibration curves. Further, it produces broadened spectral peaks because the probability of photon absorption is at a maximum near the peak maximum.

16.44
self-reversal
<GDOES> severe *self-absorption* (16.43) that produces a local minimum of intensity near the centre of a spectral peak

16.45
background equivalent concentration
<GDS> concentration of an element in a sample that would produce, in the absence of the background, a *signal intensity* (3.17) equivalent to the measured background intensity

Note 1 to entry: In *GDS* (15.1), results are often expressed in mass fractions and so the background equivalent concentration is usually expressed in these units.

16.46
preburning
presputtering
<GDS, bulk materials> process of *sputtering* (9.3), prior to signal registration, employed to allow *steady state sputtering* (9.27) to be established and analytical signals to stabilize

Note 1 to entry: Preburning is used for stabilizing the *glow discharge* (16.2).

16.47
preburn
presputtering period
<GDS, bulk materials> period during which *preburning* (16.46) occurs

Note 1 to entry: Preburning is used for stabilizing the *glow discharge* (16.2). Typical preburn times for *GDOES* (15.3) range from 30 s to 60 s, while those for *GDMS* (15.2) can be much longer.

Note 2 to entry: Glow discharge conditions used for preburn are usually identical to those employed during signal registration. However, for some applications, they can be different.

16.48
relative sensitivity factor
RSF
<GDMS> coefficient for an element by which the measured intensity of a mass peak for that element, divided by the measured intensity of a mass peak for a matrix element, is multiplied to yield the mass fraction of that element in the sample divided by the mass fraction of the matrix element

Note 1 to entry: For a given *GDMS* (15.2) instrument, the relative sensitivity factors for all elements in the periodic table usually fall within approximately one order of magnitude, making semiquantitative GDMS analysis possible without the use of *reference materials* (5.1) for calibration. However, quantitative GDMS analysis requires the use of reference materials with a matrix similar to that of the sample in order to measure the relative sensitivity factors for the elements of interest in that matrix using that particular GDMS instrument.

17 Terms related to ion scattering methods

17.1
ion beam analysis
IBA
method designed to elucidate composition and structure of the near-surface atomic layers of a solid material, in which principally monoenergetic, singly charged *probe ions* (18.1) scattered from the *surface* (3.2) are detected and recorded as a function of their energy or *angle of scattering* (8.4), or both

Note 1 to entry: *LEIS* (17.2), *MEIS* (17.3), and *RBS* (17.4) are all forms of IBA in which the probe ion energies are typically in the ranges 0,1 keV to 10 keV, 100 keV to 200 keV, and 1 MeV to 2 MeV, respectively. These classifications represent three ranges in which fundamentally different physics is involved.

17.2
low-energy ion scattering spectrometry
ion scattering spectroscopy
LEIS
ISS

method designed to elucidate composition and structure of the very outermost atomic layers of a solid material, in which principally monoenergetic, singly charged *probe ions* (18.1) scattered from the *surface* (3.2) are detected and recorded as a function of their energy or *angle of scattering* (8.4), or both

Note 1 to entry: LEIS is a form of *IBA* (17.1) in which the probe ions, typically He or Ne, have energies in the range 0,1 keV to 10 keV.

Note 2 to entry: The acronym LEIS occasionally is written LEISS.

17.3
medium-energy ion scattering spectrometry
MEIS

method designed to elucidate composition and structure of the outermost atomic layers of a solid material, in which principally monoenergetic, singly charged *probe ions* (18.1) scattered from the *surface* (3.2) are detected and recorded as a function of their energy or *angle of scattering* (8.4), or both

Note 1 to entry: MEIS is a form of *IBA* (17.1) in which the probe ions, typically protons, have energies in the range 100 keV to 200 keV.

Note 2 to entry: By using *channelling* (18.18) and aligning the incident-*ion beam* (8.8) along a crystal axis, the scattering from the substrate can be suppressed so that enhanced signal quality and visibility are obtained for amorphous overlayers. By further aligning the detector along a second crystal axis, the double-alignment mode, the scattering from the substrate can be further suppressed, improving the signal quality and visibility for amorphous overlayers to a high level.

Note 3 to entry: In some cases, an angle-sensitive detector is used that allows extensive structure and *depth profile* (3.32) information to be obtained.

Note 4 to entry: The acronym MEIS occasionally is written MEISS.

17.4
Rutherford backscattering spectrometry
RBS

method designed to elucidate composition and structure of layers at the *surface* (3.2) of a solid material, in which principally monoenergetic, singly charged *probe ions* (18.1) scattered from the surface with a *Rutherford cross section* (4.14) are detected and recorded as a function of their energy or *angle of scattering* (8.4), or both

Note 1 to entry: RBS is a form of *IBA* (17.1) in which the probe ions, typically He but sometimes H, have energies in the range 1 MeV to 2 MeV. In its traditional form, a solid-state energy-dispersive detector is used. In the form of high-resolution RBS, the energy can be reduced to 300 keV and a high-resolution (ion optical) spectrometer can be used.

Note 2 to entry: By using *channelling* (18.18) and aligning the incident- *ion beam* (8.8) along a crystal axis, the scattering from the substrate can be suppressed so that enhanced signal quality and visibility are obtained for amorphous overlayers.

17.5
direct recoil spectroscopy
DRS
elastic recoil detection
ERD
elastic recoil detection analysis
ERDA
method to elucidate composition and structure of the outermost atomic layers of a solid material, in which principally monoenergetic neutral atoms or singly charged *probe ions* (18.1) are used to *sputter* (9.3) atoms or ions out of the solid surface, their energy being recorded at one or more *angle of scattering* (8.4)

Note 1 to entry: See *Rutherford backscattering spectrometry* (17.4).

Note 2 to entry: In the analysis, it is assumed that the recoiled atom or ion is from a single *binary elastic scattering* (4.1) event. The energy is the complement of the primary ion scattered ion energy.

Note 3 to entry: By a suitable choice of scattering angle, the scattered *primary ions* (20.26) can be removed from the spectrum.

Note 4 to entry: This method is often combined with Rutherford backscattering spectrometry as they share many concepts and instrumental items.

17.6
particle-induced X-ray emission
PIXE
method in which the energies and intensities of X-rays emitted from a solid surface, under the action of a beam of atoms or ions, are detected

Note 1 to entry: Unlike electron microprobe X-ray analysis, where the generating radiation is an electron beam, in PIXE the X-ray background is much reduced so that the *detection limits* (3.9) are significantly improved while *spatial resolution* (10.14) can be maintained.

18 Terms related to ion scattering analysis

18.1
probe ion
ionic species intentionally produced by an ion source and directed onto the sample *surface* (3.2) at a known *angle of incidence* (8.1) and a known energy

18.2
target
<EIA, RBS> sample under investigation

18.3
thick target
<EIA, RBS> sample whose thickness produces backscattered particles whose energies, for each constitutive element, vary greatly with respect to the *spectrometer resolution* (10.6)

18.4
thin target
<EIA, RBS> sample whose thickness is sufficiently small that the variation in energy of particles backscattered from atoms of each constitutive element is small with respect to the *spectrometer resolution* (10.6)

18.5
scattered ion
<ISS> *probe ion* (18.1) redirected towards the detecting system after a collision with a sample atom

18.6
swift ion

ion moving with a velocity exceeding the Bohr speed of $c/137$ where c is the velocity of light

Note 1 to entry: For argon and gold, this criterion requires energies greater than 1 MeV and 5 MeV, respectively.

18.7
heavy particle

<ion analysis> particle heavier than an electron

Note 1 to entry: See *heavy ion* (3.41).

Note 2 to entry: The usage is that of the ion physics community and elsewhere the meaning can be different.

18.8
binary elastic scattering peak

<ISS> detected signal which can be attributed to *binary elastic scattering* (4.1) of an incident ion by a surface atom of a particular mass

18.9
energy edge

<ISS, RBS> values of the *backscattering energy* (4.4) for an element, or for an isotope, that is located at the *surface* (3.2) of the sample

18.10
surface approximation energy

<ISS, RBS> simplification of calculations involving the energy of an ion passing through a solid sample, where the energy of the ion at the *surface* (3.2) is used in place of a properly averaged energy

Note 1 to entry: This approximation is used to determine the energy at which scattering or *stopping cross sections* (4.11), or both, are evaluated.

18.11
stopping cross section factor

<ISS, RBS> quotient of the total *energy loss* (4.3) of a particle scattered at a given depth in the sample, and detected at a given angle, by the product of the atomic density of the sample atoms and the depth of scattering

18.12
backscattering coefficient

backscattering yield

<RBS> quotient of the number of detected particles in an interval of *backscattering energy* (4.4) by that interval and by the number of incident ions

18.13
scattered ion energy

<ISS> *kinetic energy* (3.35) of a *scattered ion* (18.5)

Note 1 to entry: Following *binary elastic scattering* (4.1), the kinetic energy of the primary or *probe ions* (18.1), E_s, is given by

$$E_s = E_0 \left[M_0 / (M_0 + M_1) \right]^2 \left\{ \cos\theta + \left[(M_1 / M_0)^2 - \sin^2\theta \right]^{\frac{1}{2}} \right\}^2$$

where

E_s is the kinetic energy of the scattered probe ion;

E_0 is the kinetic energy of the incident probe ion prior to scattering;

M_0 is the mass of the probe ion;

M_1 is the mass of the target atom;

θ is the angle between the initial and final velocity vectors for the probe ion, as determined from a common origin in the laboratory coordinate system, expressed as a value between 0° and 180°.

18.14
scattered ion energy ratio
<ISS> ratio of the *scattered ion energy* (18.13) to the energy of the incident *probe ion* (18.1) prior to a collision

18.15
kinematic factor
<RBS, ISS> ratio of the projectile energy after an elastic collision to that before the collision in the laboratory frame of reference

Note 1 to entry: The symbol K is often used for the kinematic factor and may have a subscript added in *ISS* (17.2) or *RBS* (17.4) measurements, denoting the target atom as either, say, K_{Si} or K_{28}. The subscript for atomic mass is preferred since the isotope is correctly identified.

18.16
experimental scattered ion intensity
<ISS> measured response of the energy filtering and detection system as a consequence of bombarding the sample material with an *ion beam* (8.8), usually presented as the ordinate of an *ion scattering spectrum* (18.23)

18.17
theoretical scattered ion intensity
<ISS> calculated intensity for the *probe ions* (18.1) scattered into a specified solid angle at a given direction

Note 1 to entry: For *binary elastic scattering* (4.1), the scattered-ion intensity is defined by

$$I_i(\theta) = I_0 N_i P_i \alpha_i (\mathrm{d}\sigma_i / \mathrm{d}\Omega)\theta \, \Delta\Omega T$$

where

$I_i(\theta)$ is the scattered-ion intensity from atoms of species i at a given *angle of scattering* (8.4), θ, in ions·per second;

I_0 is the intensity of incident probe ions, in ions·per second;

N_i is the number of scattering centres of species i per unit area of *surface* (3.2) accessible to the incident beam, in atoms·per square metre;

P_i is the probability that the probe ion remains ionized after interacting with an atom of species i;

α_i is the geometric or shadowing factor for species i in the given environment and geometry;

$(d\sigma_i/\mathrm{d}\Omega)\theta$ is the *differential elastic scattering cross section* (4.9) for species i, taken at the angle for which scattering is measured, i.e. the angular distribution of the scattered-ion intensity per unit *flux* (8.18) of incident ions per atom of species i, in square metres·per atom·per steradian;

$\Delta\Omega$	is the solid angle of acceptance, determined by the entrance of the filtering and detection system, in sr;
T	is the fractional transmission of the analysing and detection system.

18.18
channelling
preferential motion of energetic particles along the crystal axes of a crystalline solid as the particles move through the sample

Note 1 to entry: In *IBA* (17.1), for ion or atom motion aligned with the strings of atoms of a single crystal, the part of the beam that strikes the first atom of a string scatters (giving a "surface peak"), but the rest of the beam can go through the "empty" spaces of the crystal without direct scattering. The small-angle collisions that the fast particles have with the channel walls mostly focus the beam into the channels. Thus, the channelling yield can be as low as 1 % of the full, non-aligned, yield. Channelling is sensitive to off-lattice-site atoms and can be used to evaluate strain as well as amorphous overlayers and depth distributions of point defects (direct scattering centres), provided that the number of these atoms or defects is comparable to the channelling yield. It is also sensitive to line defects, which often do not have a large direct scattering effect but can cause substantial subsequent dechannelling deeper in the crystal. In these cases, the point defect concentrations have to be greater than about 1 atomic % and the dislocation densities greater than about 10^{11} per square centimetre.

18.19
blocking geometry
<ISS, RBS> experimental arrangement wherein the atom rows or planes of a single-crystal *target* (18.2) are aligned parallel to a vector from the sample to the detector

18.20
ion scattering spectrometer
<ISS> instrument capable of generating a *primary beam* (8.10) of principally monoenergetic, singly charged, low-energy ions and determining the energy distribution of the *primary ions* (20.26) that have been scattered from a solid *surface* (3.2) through a known angle

Note 1 to entry: For applications in surface chemical analysis, the primary ions are commonly of rare-gas atoms with energies in the range 0,1 keV to 10 keV.

18.21
solid angle of detector
<RBS> solid angle intercepted by the detector from an origin at the centre of the beam spot

18.22
pileup
<MEIS, RBS> *counts* (3.18) in a *backscattering spectrum* (18.24) arising from two or more separate events that occur so closely in time that the signals are not resolved by the detection system and cause counts to be recorded in erroneous channels

Note 1 to entry: See *dead time* (7.17).

18.23
ion scattering spectrum
<ISS> plot of the intensity of ions, scattered from a sample, as a function of the ratio of the *scattered ion energy* (18.13) to the incident-ion energy

18.24
backscattering spectrum
<RBS> plot of *backscattering yield* (18.12) versus *backscattering energy* (4.4)

18.25
aligned incidence spectrum
<EIA, ISS> *backscattering spectrum* (18.24) recorded with the analysing beam aligned with crystallographic axes or planes of the sample that produce *channelling* (18.18)

18.26
random incidence spectrum
<EIA, ISS> *backscattering spectrum* (18.24) recorded with the analysing beam incident on the sample in a direction such as to produce no *channelling* (18.18)

19 Terms related to surface mass spectrometry methods

19.1
secondary-ion mass spectrometry
SIMS
method in which a mass spectrometer is used to measure m/z (20.1) and abundance of *secondary ions* (20.28) emitted from a sample as a result of bombardment by energetic ions

Note 1 to entry: See *dynamic SIMS* (19.4), *static SIMS* (19.3), and *G-SIMS* (19.5).

19.2
secondary neutral mass spectrometry
SNMS
method in which a mass spectrometer is used to measure m/z (20.1) and abundance of post-ionized secondary neutral species emitted from a sample as a result of particle bombardment

Note 1 to entry: The neutral species can be detected by using *plasma* (16.1), electron, or photon-ionization methods.

19.3
static SIMS
SIMS (19.1) in which the *primary ion* (20.26) *dose* (8.20) is kept low enough that the original surface is altered to an insignificant extent during the experiment

Note 1 to entry: See dynamic *SIMS* (19.4).

Note 2 to entry: For static conditions the primary ion dose should be small compared to the reciprocal of the *disappearance cross section* (20.16). A typical limiting value for dose is 10^{17} ions per square metre, with dependence on the material of the sample, the *primary ion beam* (8.10) and the size of the *molecular fragments* (20.25) being analysed.

19.4
dynamic SIMS
SIMS (19.1) in which the material *surface* (3.2) is *sputtered* (9.3) at a sufficiently rapid rate that the original surface cannot be regarded as undamaged during the analysis

Note 1 to entry: Dynamic SIMS is often simply termed SIMS.

Note 2 to entry: The ion *areic dose* (8.20) during measurement is usually more than 10^{16} ions per square metre.

19.5
G-SIMS
variant of *static SIMS* (19.3) in which the intensities for each mass in two spectra from the same area, recorded with different beam energies or different bombarding ions, are ratioed to each other and the result is used to scale one of the spectra to generate a new spectrum

Note 1 to entry: As with static SIMS, the ion *areic dose* (8.20) during measurement is restricted to less than 10^{16} ions per square metre to an extent that depends on both the material of the sample and the size of the *molecular fragments* (20.25) being analysed.

Note 2 to entry: The G-SIMS spectrum enables the mass of whole molecules on the *surface* (3.2) to be determined more readily than in static SIMS.

Note 3 to entry: The “G” in G-SIMS originally indicated the gentleness of the process generated.

19.6
G-SIMS-FPM
G-SIMS with fragmentation pathway mapping
development of *G-SIMS* (19.5) in which the *g index* (20.64) is varied in order to deduce the linkages between *daughter ions* (20.33) and *parent ions* (20.32)

19.7
FAB-SIMS
<SIMS> *SIMS* (19.1) in which the *primary-ion beam* (8.10) is replaced by a fast-atom beam

19.8
fast atom bombardment mass spectrometry
FABMS
method in which a mass spectrometer is used to measure m/z (20.1) and abundance of *secondary ions* (20.28) emitted from a sample in a liquid matrix as a result of the bombardment by fast neutral atoms

19.9
matrix-assisted laser desorption/ionization mass spectrometry
MALDI
method in which a *time of flight* (20.49) mass spectrometer is used to measure m/z (20.1) and abundance of ions emitted, as a result of a short pulse of laser illumination, from a sample whose *analyte* (3.4) is contained in an ion-assisting matrix

Note 1 to entry: The matrix used for assisting the ion emission requires a strong absorbance at the laser wavelength and a low enough mass to be sublimable. Examples of matrices for 337 nm wavelength laser light are 2,5-dihydroxybenzoic acid (DHB), 3,5-dimethoxy-4-hydroxycinnamic acid (sinapinic acid), and α-cyano-4-hydroxycinnamic acid (CHCA).

Note 2 to entry: MALDI is used to analyse non-volatile polar biological and organic macromolecules as well as polymers to masses of over 3 000 kDa.

19.10
surface-assisted laser desorption/ionization
SALDI
MALDI (19.9) using a combined liquid and particulate matrix

Note 1 to entry: The particulate matrix is often graphite.

19.11
matrix-assisted laser desorption electrospray ionization
MALDESI
method in which a mass spectrometer is used to measure m/z (20.1) and abundance of ionized entities from a sample that has been mixed with a matrix whose role is enhancing the ion yield produced by laser ablation and electrospray ionization

Note 1 to entry: See *DAPPI* (19.16), *DESI* (19.12), *EESI* (19.21), and *ELDI* (19.20).

Note 2 to entry: The matrix, e.g. glycerol, allows efficient absorption of the laser energy and assists the desorption of the *analyte* (3.4) molecules in the ejected charged droplets.

Note 3 to entry: Both positive and negative ions are observed.

19.12
desorption electrospray ionization
DESI
method in which a mass spectrometer is used to measure m/z (20.1) and abundance of ionized entities emitted from a sample in air as a result of the bombardment by ionized solvent droplets generated by pneumatically assisted electrospray ionization

Note 1 to entry: Water and methanol are often used as the solvents to create the droplets. Acids and alkalis are added to control the solution pH.

Note 2 to entry: DESI is one of the few surface analysis methods designed to analyse materials without exposure to vacuum. It is used for complex molecules, organic molecules, and biomolecules. In vivo analysis is claimed to be possible.

19.13

reactive DESI

mode of *DESI* (19.12) with reactive chemicals within the spray solution to enhance the analytical specificity

19.14

direct analysis in real time

DART

method in which a mass spectrometer is used to measure *m/z* (20.1) and abundance of ionized entities emitted from a sample in air as a result of the interaction with a beam containing metastable, excited atoms heated to ~500 °C

Note 1 to entry: See *DAPCI* (19.17) and *PADI* (19.15).

Note 2 to entry: DART is the registered trademark of JEOL, USA, Inc. This information is given for the convenience of users of this document and does not constitute an endorsement by ISO of the product named. Equivalent products can be used if they can be shown to lead to the same results.

Note 3 to entry: The beam atoms usually used are helium, nitrogen, or neon.

Note 4 to entry: Both positive and negative ions are observed although the mechanism for positive ions can be through protonation involving water molecules and the process for negative ions through *Penning ionization* (16.30).

19.15

plasma-assisted desorption ionization

PADI

method in which a mass spectrometer is used to measure *m/z* (20.1) and abundance of ionized entities emitted from a sample in air as a result of the bombardment by a focused *plasma* (16.1)

Note 1 to entry: See *DART* (19.14) and *DAPCI* (19.17).

Note 2 to entry: The energy of the plasma ions is very low.

Note 3 to entry: The plasma gas is usually helium, nitrogen, air, or argon.

Note 4 to entry: Both positive and negative ions are observed although the mechanism for positive ions can be through protonation involving water molecules and the process for negative ions through *Penning ionization* (16.30).

19.16

desorption atmospheric pressure photoionization

DAPPI

method in which a mass spectrometer is used to measure *m/z* (20.1) and abundance of ionized entities emitted from a sample in air as a result of desorption by a jet of hot solvent vapour and ionization by ultraviolet light

Note 1 to entry: See *DESI* (19.12), *EESI* (19.21), *ELDI* (19.20), *LAESI* (19.19), and *MALDESI* (19.11).

Note 2 to entry: The desorption mechanism is thermal.

Note 3 to entry: Both positive and negative ions are observed.

19.17
desorption atmospheric pressure chemical ionization

DAPCI

method in which a mass spectrometer is used to measure *m/z* (20.1) and abundance of ionized entities emitted from a sample in air as a result of a nearby corona discharge in a carrier gas

Note 1 to entry: See *DART* (19.14) and *PADI* (19.15).

Note 2 to entry: The carrier gas is usually nitrogen.

Note 3 to entry: Both positive and negative ions are observed with the mechanisms involving protonation through water molecules and ionization through the Penning process.

19.18
laser desorption ionization

LDI

method in which a mass spectrometer is used to measure *m/z* (20.1) and abundance of ionized entities emitted from a sample as a result of laser ablation

19.19
laser ablation electrospray ionization

LAESI

method in which a mass spectrometer is used to measure *m/z* (20.1) and abundance of ionized entities emitted from a sample in air as a result of laser ablation and electrospray ionization

Note 1 to entry: See *DAPPI* (19.16), *DESI* (19.12), *EESI* (19.21), *ELDI* (19.20), and *MALDESI* (19.11).

Note 2 to entry: The laser wavelength is usually in the infrared region.

Note 3 to entry: Both positive and negative ions are observed with the mechanisms involving protonation through water molecules and ionization through the Penning process.

19.20
electrospray laser desorption ionization mass spectrometry

ELDI

method in which a mass spectrometer is used to measure *m/z* (20.1) and abundance of ionized entities emitted from a sample in air via ablation by a focused pulsed laser while simultaneously directing an electrospray jet through the desorbed plume to enhance sample ionization

Note 1 to entry: See *DAPPI* (19.16), *DESI* (19.12), *EESI* (19.21), *LAESI* (19.19), and *MALDESI* (19.11).

Note 2 to entry: The desorption mechanism is thermal.

Note 3 to entry: Both positive and negative ions are observed.

Note 4 to entry: With the addition of a matrix on the sample, this is termed matrix-assisted laser desorption electrospray ionization (MALDESI).

Note 5 to entry: With the use of an infrared laser for ablation, this has sometimes been termed laser ablation electrospray ionization (LAESI).

19.21
extractive electrospray ionization

EESI

method in which a mass spectrometer is used to measure *m/z* (20.1) and abundance of ionized entities emitted from a sample in air as a result of an inert gas being passed over the sample to pick up the molecules which are subsequently ionized by ionized solvent droplets generated by pneumatically assisted electrospray ionization

Note 1 to entry: See *DAPPI* (19.16), *DESI* (19.12), *ELDI* (19.20), *LAESI* (19.19), and *MALDESI* (19.11).

Note 2 to entry: Both positive and negative ions are observed.

20 Terms related to surface mass spectrometry analysis

20.1

mass-to-charge ratio

m/*z*

the positive absolute value of the quantity formed by dividing the mass of an ion by the *unified atomic mass unit* (3.6) and by its charge number

20.2

nominal mass

particle mass, in *unified atomic mass units*, *u* (3.6), rounded to the nearest integer

20.3

degree of ionization

<SIMS, FABMS> quotient of the number of ions of a species emitted by the number of *sputtered* (9.3) particles of that species

20.4

sputtering yield

ratio of the number of atoms and ions *sputtered* (9.3) from a sample to the total number of incident primary particles

20.5

fractional sputtering yield

ratio of the number of atoms and ions of a particular species sputtered from a sample to the total number of atoms and ions sputtered from the sample

Note 1 to entry: See *fractional ion yield* (20.13), *negative-ion yield* (20.10), *partial ion yield* (20.12), *partial sputtering yield* (20.6), *positive-ion yield* (20.11), and *total ion yield* (20.7).

20.6

partial sputtering yield

ratio of the number of atoms and ions of a particular species sputtered from a sample to the total number of incident particles

Note 1 to entry: See *fractional ion yield* (20.13), *fractional sputtering yield* (20.5), *negative-ion yield* (20.10), *partial ion yield* (20.12), *positive-ion yield* (20.11), and *total ion yield* (20.7).

20.7

total ion yield

ratio of the total number of ions of both signs sputtered from a sample to the total number of incident particles

Note 1 to entry: See *fractional ion yield* (20.13), *fractional sputtering yield* (20.5), *negative-ion yield* (20.10), *partial ion yield* (20.12), *partial sputtering yield* (20.6), and *positive-ion yield* (20.11).

Note 2 to entry: The total ion yield is often used where, more correctly, the writer means the total negative-ion yield or the total positive-ion yield rather than their sum.

20.8

secondary-ion yield

ratio of the total number of ions *sputtered* (9.3) from a sample to the total number of ions incident with a given mass, energy, charge, and *angle of incidence* (8.1)

20.9

secondary-electron yield

secondary-electron emission coefficient

<GDS, SIMS> ratio of the total number of electrons emitted from a sample to the total number of particles incident upon the sample *surface* (3.2)

Note 1 to entry: Secondary-electron yield is sometimes given for a particular type of energetic incident particle such as Ar^+.

20.10

negative ion yield

ratio of the total number of negative *secondary ions* (20.28) sputtered from a sample to the total number of incident primary particles

Note 1 to entry: See *fractional ion yield* (20.13), *partial ion yield* (20.12), and *total ion yield* (20.7).

20.11

positive ion yield

ratio of the total number of positive *secondary ions* (20.28) sputtered from a sample to the total number of incident primary particles

Note 1 to entry: See *fractional ion yield* (20.13), *partial ion yield* (20.12), and *total ion yield* (20.7).

20.12

partial ion yield

partial ion sputtering yield

ratio of the number of ions of a particular species sputtered from a sample to the total number of incident particles

Note 1 to entry: See *fractional ion yield* (20.13), *fractional sputtering yield* (20.5), *negative-ion yield* (20.10), *partial sputtering yield* (20.6), *positive-ion yield* (20.11), and *total ion yield* (20.7).

20.13

fractional ion yield

ratio of the number of ions of a particular species sputtered from a sample to the total number of particles of that species sputtered from that sample

Note 1 to entry: See *fractional sputtering yield* (20.5) and *partial sputtering yield* (20.6).

20.14

useful ion yield

<SIMS> ratio of the number of ions of a particular isotope detected to the total number of atoms of the same element sputtered from the sample

20.15

dilute limit

<SIMS> atomic fraction or concentration of impurity species in a homogeneous matrix below which the SIMS process can safely be assumed to be linear with composition

20.16

disappearance cross section

<SIMS> *cross section* (4.7) for the loss of intensity of an ion signal observed as a result of the bombardment by *primary ions* (20.26)

Note 1 to entry: See *damage cross section* (4.27).

Note 2 to entry: The ion signal used is usually that for a large or characteristic fragment of the molecule, such as a *cationized* (20.22), *protonated molecules* (20.20), or *deprotonated molecule* (20.21) from the molecule, at a *surface* (3.2).

Note 3 to entry: Disappearance implies that no signal of a species under consideration can be detected from this area in further experiments. The respective material can either be desorbed from the surface by the experiment or remain in a fragmented or damaged state on the surface.

20.17

efficiency

<SIMS> quotient of the measured yield of an *ion species* (3.36) per *primary ion* (20.26) and the *disappearance cross section* (20.16)

Note 1 to entry: See *ionization efficiency* (3.45).

20.18
polyatomic ion
charged multi-atom species

Note 1 to entry: Dimer and trimer ions are specific examples of polyatomic ions containing two and three atoms, respectively.

20.19
molecular ion
ion formed by the removal from (positive ions) or addition to (negative ions) a molecule of one or more electrons without *fragmentation* (20.23) of the molecular structure

[SOURCE: IUPAC]

Note 1 to entry: *Protonated molecules* (20.20) and *deprotonated molecules* (20.21) are often of greater intensity than the *molecular ion* (20.19) in SIMS, MALDI and ambient surface mass spectrometry.

20.20
protonated molecule
molecule to which a proton has been added to form a positive ion

20.21
deprotonated molecule
molecule from which a proton has been removed to form a negative ion

20.22
cationized molecule
positively charged ion resulting from a neutral molecule combining with a *cation* (3.43)

Note 1 to entry: Cationization is a common ionization mechanism in the analysis of monomolecular layers on noble metal substrates in *static SIMS* (19.3). There, a cation from the substrate (e.g. Ag^+) leads to the formation of a $(M+Ag)^+$ quasi-molecular ion. From thicker layers, cationization by ions from salts is observed [e.g. $(M+Na)^+$].

20.23
fragmentation
breakdown of a molecule or ion to form one or more ions or neutral species of lower mass whilst conserving the total charge

20.24
polyatomic fragment
ion or neutral particle composed of three or more atoms

20.25
molecular fragment
ion or neutral particle that was part of a larger molecular structure and contains information about that structure

20.26
primary ion
ion extracted from a source and directed at a sample

Note 1 to entry: See *probe ion* (18.1) and *secondary ion* (20.28).

20.27
transformation probability
<SIMS> probability of a defined charged or neutral species being produced, by consumption of a defined parent atomic or molecular configuration at a *surface* (3.2), as a result of *sputtering* (9.3)

20.28
secondary ion
ion ejected from a sample *surface* (3.2) as a result of energy and momentum transfer from a *primary ion* (20.26)

20.29

secondary-ion angular distribution

number of *secondary ions* (20.28) as a function of *angle of emission* (8.5)

20.30

secondary-ion energy distribution

number of *secondary ions* (20.28) as a function of their *kinetic energy* (3.35) at a specified collection angle

20.31

fragment ion

charged dissociation product arising from ionic *fragmentation* (20.23)

[SOURCE: IUPAC]

Note 1 to entry: See *daughter ion* (20.33) and *metastable ion* (20.34).

Note 2 to entry: Fragment ions can dissociate further to form other electrically charged molecular or atomic moieties of successively lower mass.

20.32

parent ion

precursor ion

ion that subsequently fragments into smaller ions or neutral particles

20.33

daughter ion

product ion

electrically charged product formed from a *parent ion* (20.32) or from a neutral entity generally of a larger size

Note 1 to entry: Formation of the product does not necessarily involve *fragmentation* (20.23). It can, for example, involve a change in the number of charges carried. Thus, all *fragment ions* (20.31) are daughter ions, but not all daughter ions are necessarily fragment ions.

20.34

metastable ion

ion that spontaneously fragments between emission and detection

Note 1 to entry: See *metastable background* (20.36).

20.35

unimolecular dissociation

spontaneous dissociation of a molecule into two or more fragments

Note 1 to entry: This term is often applied to the *fragmentation* (20.23) of a *metastable ion* (20.34).

20.36

metastable background

<SIMS> intensity in the *mass spectrum* (20.58) arising from ions that spontaneously fragment between emission and detection

Note 1 to entry: In *reflectron* (20.50) *time of flight* (20.49) mass spectrometers, the decay of *metastable ions* (20.34) leads to broad peaks at a mass dependent on the drift energy and *reflector voltage* (20.52). Good design minimizes these *background signals* (3.21).

20.37

mass analyser

device for dispersing and detecting particles as a function of their *mass-to-charge ratio* (20.1)

20.38
cluster SIMS

<SIMS> *SIMS* (19.1) utilizing a *primary beam* (8.10) composed of *cluster ions* (3.44)

Note 1 to entry: Cluster ion sources are often used in *static SIMS* (19.3) to enhance molecular signals and in *dynamic SIMS* (19.4) to enhance *depth resolution* (10.18).

20.39
extraction field

<SIMS> electric field above the sample, operational during ion emission from the sample

Note 1 to entry: The extraction field can be pulsed or constant, depending on the type of instrument.

20.40
extractor voltage

<SIMS> voltage, referenced to the sample, of the electrode defining the field above the sample and used to facilitate the introduction of emitted ions into the mass spectrometer

Note 1 to entry: This voltage, together with the separation distance between the sample and the extractor electrode, defines the *extraction field* (20.39).

20.41
extraction bias

<SIMS> voltage between the electrodes used to define the *extraction field* (20.39) occurring in the period between ion pulses in the pulsed-extraction mode

Note 1 to entry: This term is used in *time of flight* (20.49) SIMS instruments.

Note 2 to entry: The extraction bias can be set to zero or it can be set at a particular value to deflect low-energy electrons to the sample for *charge neutralization* (8.45) or, in dual-ion-beam systems for *depth profiling* (3.34), to deflect *secondary ions* (20.28) generated by the *sputter depth profiling* (9.1) ion gun in order to prevent them from entering the mass spectrometer and generating background *counts* (3.18).

20.42
pulsed extraction field

<SIMS> *extraction field* (20.39) around the sample that is pulsed to the working value for extracting ions for the time necessary for operation of a *time of flight* (20.49) mass spectrometer but is otherwise at a low value

Note 1 to entry: This is the usual mode in *time of flight* (20.49) *SIMS* (19.1) systems either for studying insulators, where the *charge neutralization* (8.45) is established while the extraction field is off, or for *depth profiling* (3.34) using a second *ion beam* (8.8) while the extraction field is off.

20.43
post-ionization

<APT, SIMS, SNMS, MALDI> mechanism through which ions or atoms are ionized to a higher absolute charge number after emission from a surface

20.44
beam bunching

<SIMS> reduction in the spread of arrival times of an ion pulse by reduction in the speed of the leading ions or acceleration of those at the trailing edge of the pulse

Note 1 to entry: See *beam blanking* (7.22) and *beam chopper* (20.48).

Note 2 to entry: This procedure can degrade the optimum focus of the *ion beam* (8.8) since different ions experience different fields.

20.45
buncher
device to shorten the time length of a pulse of ions so that they arrive at a point over a reduced time interval

Note 1 to entry: The point is usually the sample surface.

20.46
dual-beam profiling
<SIMS> *sputter depth profiling* (9.1) involving two ion guns

Note 1 to entry: Two similar ion guns can be used in opposite azimuths of the sample to reduce the development of topography.

Note 2 to entry: In *time of flight* (20.49) mass spectrometers, one beam is used with a short on-time for the *SIMS* (19.1) analysis while a second is used during the period when the first is off and the mass analysis has been completed in each cycle. The second gun provides the ions for sputter removal of the sample to form the *depth profile* (3.32). This combination allows practical *sputtering rates* (9.19) to be achieved and the profiling to be optimized separately from the optimization for the SIMS analysis.

20.47
analyser blanking
<SIMS> action to prevent *secondary ions* (20.28) from travelling through the mass spectrometer and being detected

20.48
beam chopper
<SIMS> electrostatic or electromagnetic device used to generate pulses of ions from a continuous *ion beam* (8.8)

Note 1 to entry: See *beam blanking* (7.22) and *beam bunching* (20.44).

Note 2 to entry: The beam chopper can be used to define the pulse length and hence the *mass resolution* (10.25) in a *time of flight* (20.49) mass spectrometer and it can also be used to select particular ions in a beam that contains more than one species.

20.49
time of flight
TOF
ToF
<SIMS> total time taken for ions of a particular mass to move from the sample to the detector

Note 1 to entry: Usually, the clock timer is started with the *beam chopper* (20.48) sequence selecting an ion pulse, and so the recorded flight time can include the additional time for the *primary ion* (20.26) to travel to the sample *surface* (3.2) from the pulse-forming region of the ion gun.

20.50
reflectron
<SIMS> *time of flight* (20.49) mass spectrometer in which ions are reflected through an angle approaching 180° in order to reduce the flight time dependence on the particular energy of the ions

20.51
stop event
<SIMS> registration of a particle by a time-to-digital converter

Note 1 to entry: The arrival time for each ion providing a pulse at the detector is registered by the time-to-digital converter (TDC). This is a stop event. TDCs may only record a fixed number of stop events during the time following each primary-ion pulse, for example 512 or 1 024, other events being lost.